Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information: Excitation Localization/Delocalization Induced Intramolecular Singlet Fission in Cyclopentadithiophene-Based Quinoidal Derivatives

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Synthesis process of QP2 and QT2

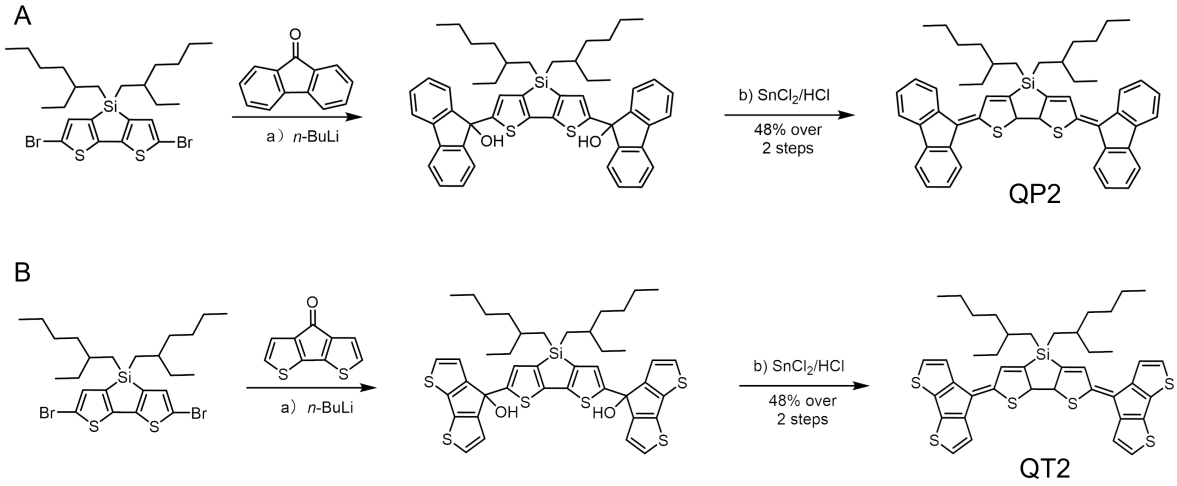


Figure S1: Synthesis process of QP2 (a) and QT2 (b).

QP2: ^{1}H NMR (chloroform-*d*, 600 MHz, δ/ppm): 8.13 (d, J = 7.7, 2H), 8.02-7.94 (m, 4H), 7.81-7.79 (m, 4H), 7.46-7.29 (m, 8H), 1.69-1.61 (m, 2H), 1.49-1.08 (m, 20H), 0.95-79 (m, 12H).

^{13}C NMR (chloroform-*d*, 150 MHz, δ/ppm): 154.62, 149.60, 148.45, 139.70, 139.36, 137.81, 131.88, 127.20, 127.06, 124.35, 123.42, 120.14, 119.97, 36.05, 36.00, 29.20, 29.03, 23.27, 18.41, 14.35, 10.94.

QT2: ^{1}H NMR (chloroform-*d*, 400 MHz, 4/ppm): 7.42 (s, 2H), 7.33-7.32 (d, J = 4, 2H), 7.25-7.24 (m, 2H), 7.12-7.11 (d, J = 4, 2H), 7.09-7.07 (d, J = 4, 2H), 1.39-1.22 (m, 16H), 1.11-1.08 (m, 4H), 0.88-0.84 (m, 14H).

^{13}C NMR (chloroform-*d*, 100 MHz, 4/ppm): 155.63, 155.60, 155.58, 149.11, 148.64, 143.44, 142.31, 136.95, 136.07, 131.42, 124.10, 124.05, 124.03, 124.01, 121.98, 121.20, 121.18, 121.15, 120.78, 35.70, 35.62, 28.81, 28.70, 22.91, 18.03, 14.01, 10.63.

Quantum yield of QP1 in DCM

We determined the quantum yield of the triplet state in QP1 in a DCM solution by comparing the differences between the measured femtosecond transient absorption (fs-TA) and triplet-sensitized spectroscopy. The transient absorption spectrum value (A) of the sample at a specific time is equal to the product of the extinction coefficient (ε) of the sample at that time, the concentration (c) of the sample at that time, and the optical path (l) of the sample.

$$A = \varepsilon c l \tag{1}$$

Hence, we can calculate the concentration when we have information about the extinction coefficient, transient absorption spectrum value, and the sample's optical path using the following equation.

$$c = A/\varepsilon l \tag{2}$$

We denote the concentrations of the triplet and singlet states of QP1 in DCM as $c(^3\mathrm{QP1}^*)$ and $c(^1\mathrm{QP1}^*)$ respectively. They can be calculated as follows.

$$c(^3\mathrm{QP1}^*) = \frac{\Delta A(^3\mathrm{QP1}^*)}{\varepsilon(^3\mathrm{QP1}^*)l} \tag{3}$$

$$c(^1\mathrm{QP1}^*) = \frac{\Delta A(^1\mathrm{QP1}^*)}{\varepsilon(^1\mathrm{QP1}^*)l} \tag{4}$$

Throughout the experimental process, we assume that the extinction coefficient at the ground-state bleaching site remains constant, representing the extinction coefficient of steady-state particles. This value remains consistent for both the singlet and triplet states, $\varepsilon(^3\mathrm{QP1}^*) = \varepsilon(^1\mathrm{QP1}^*)$, and the optical path remains unchanged. The quantum yield of the triplet state can be calculated by dividing the spectral value of the triplet state by that of the singlet state.

$$\mathrm{Yield}(^3\mathrm{QP1}^*) = \frac{c(^3\mathrm{QP1}^*)}{c(^1\mathrm{QP1}^*)} = \frac{\Delta\mathrm{A}(^3\mathrm{QP1}^*)/\varepsilon(^3\mathrm{QP1}^*)l}{\Delta\mathrm{A}(^1\mathrm{QP1}^*)/\varepsilon(^1\mathrm{QP1}^*)l} = \frac{\Delta\mathrm{A}(^3\mathrm{QP1}^*)}{\Delta\mathrm{A}(^1\mathrm{QP1}^*)}. \tag{5}$$

Excitation energies from TD-DFT and multireference calculations.

Table S1: DRC index y_0 of different compounds calculated at UHF/cc-pVDZ level.

	y_0	T	n_{HONO}	n_{LUNO}
QP1	0.368	0.356	1.356	0.644
QP2	0.395	0.337	1.337	0.663
QT1	0.301	0.408	1.408	0.592
QT2	0.329	0.385	1.385	0.614

Table S2: Vertical excitation energies of QP1 calculated at the B3LYP/cc-pVDZ level.

state	E (eV)	E (nm)	f
S_1	2.0553	603.23	1.9521
S_2	2.4766	500.63	0.0002
S_3	2.4767	500.61	0.0008
S_4	2.7375	452.91	0.0013
S_5	3.3332	371.97	0.0202
S_6	3.4411	360.30	0.0051
S_7	3.4593	358.41	0.0026
S_8	3.4757	356.72	0.0306
S_9	3.5175	352.48	0.0123
S_{10}	3.6868	336.29	0.0012
S_{11}	3.8040	325.93	0.0021
S_{12}	3.8999	317.92	0.0526
S_{13}	3.9335	315.20	0.0106
S_{14}	3.9351	315.07	0.0099
S_{15}	4.1766	296.85	0.0270
S_{16}	4.1857	296.21	0.0182
S_{17}	4.3089	287.74	0.0044
S_{18}	4.3119	287.54	0.0001
S_{19}	4.3144	287.37	0.0022
S_{20}	4.3363	285.92	0.0006
S_21	4.6011	269.46	0.0399
S_{22}	4.6134	268.75	0.0087
S_{23}	4.6724	265.36	0.2846
S_{24}	4.6737	265.28	0.0248
S_{25}	4.7564	260.67	0.0038
T_1	0.6845	1811.22	0
T_2	2.0173	614.59	0
T_3	2.2473	551.69	0
T_4	2.2475	551.66	0
T_5	2.6118	474.70	0
T_6	3.0950	400.59	0
T_7	3.1035	399.50	0
T_8	3.1319	395.88	0
T_9	3.2060	386.72	0
T_{10}	3.2421	382.41	0
T_{11}	3.2838	377.57	0
T_{12}	3.2970	376.05	0
T_{13}	3.4093	363.66	0
T_{14}	3.4295	361.53	0
T_{15}	3.7044	334.70	0
T_{16}	3.8331	323.46	0
T_{17}	3.8522	321.85	0
T_{18}	3.8526	321.82	0
T_{19}	3.9428	314.46	0
T_{20}	3.9999	309.97	0
T_21	4.0318	307.52	0
T_{22}	4.0519	305.99	0
T_{23}	4.0765	304.14	0
T_{24}	4.0998	302.42	0
T_{25}	4.3247	286.69	0

Table S3: Vertical excitation energies of QP2 calculated at the B3LYP/cc-pVDZ level.

state	E (eV)	E (nm)	f
S_1	1.9870	623.96	1.8098
S_2	2.4339	509.41	0.0001
S_3	2.4343	509.32	0.0012
S_4	2.5946	477.85	0.0001
S_5	3.1985	387.63	0.0661
S_6	3.4129	363.28	0.0050
S_7	3.4218	362.34	0.0343
S_8	3.4399	360.43	0.0014
S_9	3.4494	359.44	0.0153
S_{10}	3.6990	335.18	0.0006
S_{11}	3.6997	335.12	0.0003
S_{12}	3.7478	330.82	0.0016
S_{13}	3.7509	330.55	0.0064
S_{14}	3.8806	319.50	0.0509
S_{15}	3.9787	311.62	0.0512
S_{16}	4.0546	305.79	0.0121
S_{17}	4.2364	292.66	0.0126
S_{18}	4.2691	290.42	0.0000
S_{19}	4.2738	290.10	0.0103
S_{20}	4.3009	288.28	0.0004
S_21	4.3043	288.05	0.0002
S_{22}	4.5176	274.45	0.0727
S_{23}	4.5869	270.30	0.0274
S_{24}	4.5876	270.26	0.0917
S_{25}	4.7476	261.15	0.0094
T_1	0.5884	2107.13	0
T_2	1.9027	651.62	0
T_3	2.2085	561.38	0
T_4	2.2088	561.31	0
T_5	2.4479	506.48	0
T_6	3.0630	404.78	0
T_7	3.0739	403.35	0
T_8	3.0890	401.37	0
T_9	3.1805	389.83	0
T_{10}	3.1929	388.32	0
T_{11}	3.2390	382.78	0
T_{12}	3.2766	378.40	0
T_{13}	3.3592	369.09	0
T_{14}	3.3761	367.24	0
T_{15}	3.5973	344.66	0
T_{16}	3.7151	333.73	0
T_{17}	3.7153	333.71	0
T_{18}	3.7631	329.47	0
T_{19}	3.7944	326.75	0
T_{20}	3.9345	315.12	0
T_21	3.9363	314.98	0
T_{22}	4.0310	307.58	0
T_{23}	4.0333	307.40	0
T_{24}	4.0473	306.34	0
T_{25}	4.2091	294.56	0

Table S4: Vertical excitation energies of QT1 calculated at the B3LYP/cc-pVDZ level.

state	E (eV)	E (nm)	f
S_1	1.7942	691.01	0.0000
S_2	1.7945	690.90	0.0066
S_3	2.1333	581.19	2.0316
S_4	2.7490	451.01	0.0006
S_5	3.1926	388.35	0.0051
S_6	3.1927	388.33	0.0358
S_7	3.3918	365.54	0.0205
S_8	3.4824	356.03	0.0017
S_9	3.4945	354.80	0.0529
S_{10}	3.6223	342.28	0.0001
S_{11}	3.7325	332.17	0.0093
S_{12}	3.8304	323.69	0.0010
S_{13}	3.9241	315.96	0.0521
S_{14}	4.0296	307.68	0.0006
S_{15}	4.0657	304.95	0.0003
S_{16}	4.1422	299.32	0.0000
S_{17}	4.1470	298.97	0.0441
S_{18}	4.1664	297.58	0.0161
S_{19}	4.1701	297.32	0.2310
S_{20}	4.4148	280.84	0.0371
S_21	4.5614	271.81	0.0025
S_{22}	4.5627	271.74	0.1977
S_{23}	4.7453	261.28	0.0000
S_{24}	4.7462	261.23	0.0001
S_{25}	4.7853	259.09	0.0026
T_1	0.7392	1677.35	0
T_2	1.4920	831.00	0
T_3	1.4923	830.84	0
T_4	2.0518	604.26	0
T_5	2.6115	474.75	0
T_6	2.6605	466.02	0
T_7	2.6607	465.99	0
T_8	3.0718	403.62	0
T_9	3.1930	388.30	0
T_{10}	3.2095	386.31	0
T_{11}	3.3707	367.83	0
T_{12}	3.4085	363.75	0
T_{13}	3.4867	355.59	0
T_{14}	3.4878	355.48	0
T_{15}	3.5300	351.23	0
T_{16}	3.6098	343.47	0
T_{17}	3.6246	342.06	0
T_{18}	3.7080	334.37	0
T_{19}	3.7875	327.35	0
T_{20}	3.9595	313.13	0
T_21	4.0302	307.64	0
T_{22}	4.0693	304.68	0
T_{23}	4.2897	289.03	0
T_{24}	4.2908	288.96	0
T_{25}	4.3047	288.02	0

Table S5: Vertical excitation energies of QT2 calculated at the B3LYP/cc-pVDZ level.

state	E (eV)	E (nm)	f
S_1	1.7469	709.72	0.0000
S_2	1.7470	709.69	0.0054
S_3	2.0640	600.71	1.8818
S_4	2.6074	475.51	0.0000
S_5	3.0170	410.95	0.0231
S_6	3.0171	410.94	0.0095
S_7	3.2702	379.14	0.0642
S_8	3.4399	360.43	0.0534
S_9	3.4463	359.76	0.0001
S_{10}	3.5935	345.02	0.0000
S_{11}	3.7119	334.02	0.0002
S_{12}	3.7365	331.81	0.0038
S_{13}	3.7946	326.74	0.0024
S_{14}	3.9082	317.24	0.0538
S_{15}	3.9890	310.82	0.0737
S_{16}	3.9970	310.19	0.0054
S_{17}	4.0042	309.64	0.0000
S_{18}	4.1700	297.32	0.0332
S_{19}	4.1757	296.92	0.2376
S_{20}	4.3021	288.19	0.0299
S_21	4.3539	284.77	0.1692
S_{22}	4.3563	284.61	0.0015
S_{23}	4.6161	268.59	0.0064
S_{24}	4.6281	267.89	0.1054
S_{25}	4.6613	265.98	0.0000
T_1	0.6446	1923.47	0
T_2	1.4525	853.61	0
T_3	1.4531	853.26	0
T_4	1.9258	643.81	0
T_5	2.4775	500.44	0
T_6	2.6171	473.74	0
T_7	2.6174	473.70	0
T_8	3.0379	408.13	0
T_9	3.1309	396.00	0
T_{10}	3.1681	391.35	0
T_{11}	3.2800	378.00	0
T_{12}	3.3156	373.94	0
T_{13}	3.3181	373.66	0
T_{14}	3.3348	371.79	0
T_{15}	3.4820	356.07	0
T_{16}	3.5098	353.25	0
T_{17}	3.5660	347.68	0
T_{18}	3.5863	345.72	0
T_{19}	3.7163	333.62	0
T_{20}	3.8909	318.65	0
T_21	3.9390	314.76	0
T_{22}	4.0403	306.87	0
T_{23}	4.2559	291.32	0
T_{24}	4.2567	291.27	0
T_{25}	4.2872	289.19	0

Table S6: Adiabatic excitation energies in low-lying excited states calculated at the TD-B3LYP/cc-pVDZ level in QP1 and QT1.

	S_1^{LE}	S_1^{DE}	T_1	T_2
QP1	2.03	1.92	0.59	1.83
QT1	1.31	–	0.71	1.02

Table S7: Vertical excitation energies (in eV) of low-lying excited states in QP1 and QT1 calculated at multireference levels.

	S_1	S_2	S_3	T_1	T_2	T_3
QP1	2.135[a]	3.144	3.144	1.292	2.383	2.944
	(2.198)[b]	(3.241)	(3.241)	(1.306)	(2.416)	(3.012)
QT1	2.183[a]	2.447	2.448	1.329	2.162	2.163
	(2.336)[b]	(2.499)	(2.500)	(1.500)	(2.128)	(2.128)

[a] MS-CASPT2/cc-pVDZ (IPEA shift = 0.00 a.u.), [b] MC-PDFT/cc-pVDZ [c]

Table S8: Vertical excitation energies (in eV) calculated at the B3LYP/cc-pVDZ level of low-lying excited states with the oscillator strengths listed in the parentheses.

	S_1	S_2	S_3	T_1	T_2	T_3	ΔE_{ST}
QP1	2.055	2.477	2.477	0.685	2.017	2.247	1.370
	(1.952)	(0.000)	(0.001)	(0)	(0)	(0)	
QP2	1.987	2.434	2.434	0.588	1.903	2.209	1.399
	(1.810)	(0.000)	(0.001)	(0)	(0)	(0)	
QT1	1.794	1.795	2.133	0.739	1.492	1.492	1.055
	(0.000)	(0.007)	(2.032)	(0)	(0)	(0)	
QT2	1.747	1.747	2.064	0.645	1.453	1.453	1.102
	(0.000)	(0.005)	(1.882)	(0)	(0)	(0)	

Table S9: Vertical excitation energies (in eV) of T_1-T_n transitions calculated at the B3LYP/cc-pVDZ level in QTs and QPs.

	T_2	T_3	T_4	T_5	T_6
QP1	1.542	1.643	1.643	2.247	2.380
QP2	1.537	1.664	1.664	2.146	2.369
QT1	0.810	0.810	1.532	1.906	1.906
QT2	0.831	0.832	1.510	1.883	1.884

Table S10: The non-radiative decay rates constants (in s^{-1}) and SOC (in cm^{-1}) calculated at the B3LYP/cc-pVDZ level.

	k_{IC}	k_{ISC} ($T_1 \rightarrow S_0$)	$\langle S_0\|\hat{\mathcal{H}}_{SO}\|T_1\rangle$	k_{ISC} ($S_1 \rightarrow T_1$)	$\langle S_1\|\hat{\mathcal{H}}_{SO}\|T_1\rangle$	k_{ISC} ($S_1 \rightarrow T_2$)	$\langle S_1\|\hat{\mathcal{H}}_{SO}\|T_2\rangle$
QP1	6.3×10^{11}	–	–	7.6×10^{6}[a]	0.44[a]	1.5×10^{7}[a]	0.27[a]
QP1	3.4×10^{11}	2.0×10^{8}	6.25	7.7×10^{4}[b]	0.68[b]	7.2×10^{2}[b]	2.35[b]
QT1	1.8×10^{12}	1.5×10^{6}	0.11	6.8×10^{6}	0.31	1.5×10^{5}	0.22

[a] localized excited state S_1^{LE}.
[b] delocalized excited state S_1^{DE}.

Electronic structure and computational potential energy surfaces

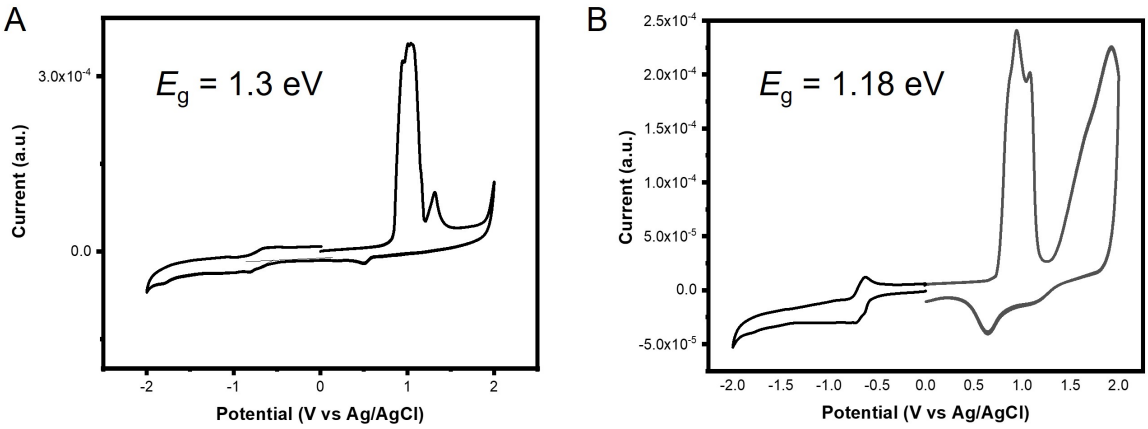


Figure S2: CV curves for QP2 (a) and QT2 (b).

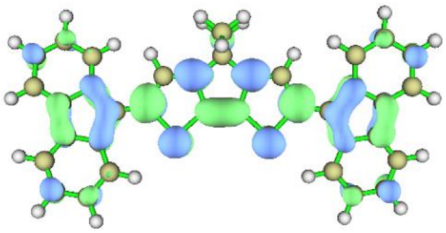
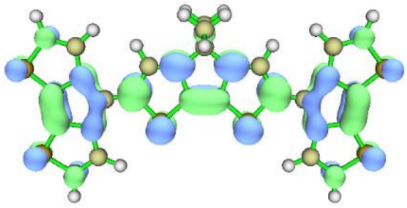
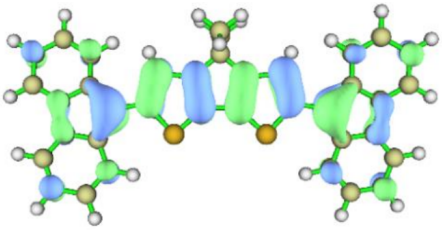
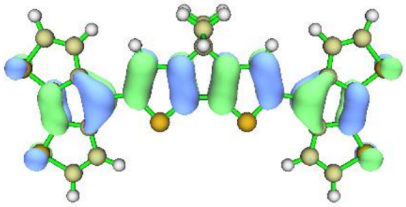
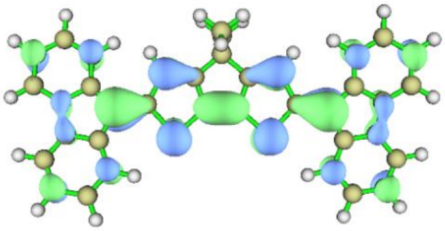
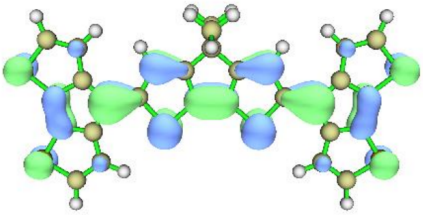
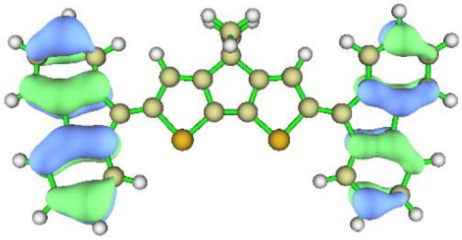
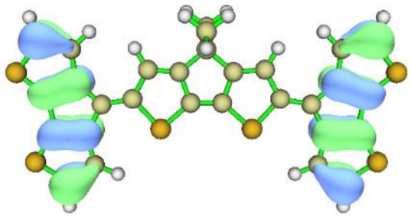
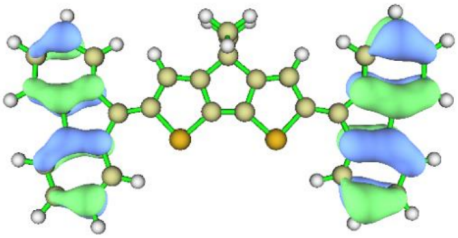
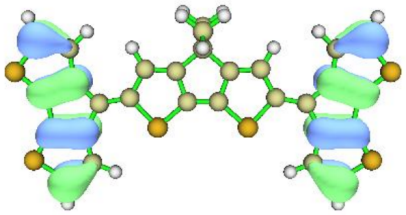
	QP1		QT1	
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
S_1	**HOMO → LUMO (98.7 %)**		**S_1**	**HOMO-2 → LUMO (98.6 %)**
			S_2	**HOMO-1 → LUMO (98.6 %)**
			S_3	**HOMO → LUMO (100 %)**
T_1	**HOMO → LUMO (96.5 %)**		**T_1**	**HOMO → LUMO (96.3 %)**

Figure S3: Frontier molecular orbitals with the isovalue of 0.03 a.u. and electronic transitions in the low-lying singlet and triplet states for QP1 and QT1 simulated at the TD-B3LYP/cc-pVDZ level.

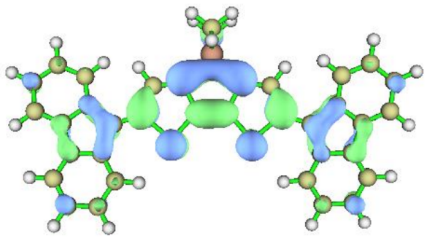
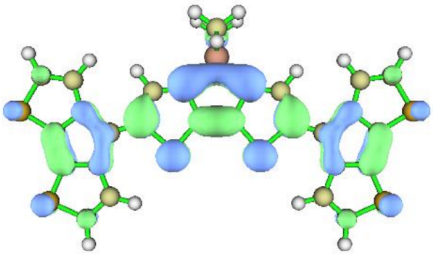
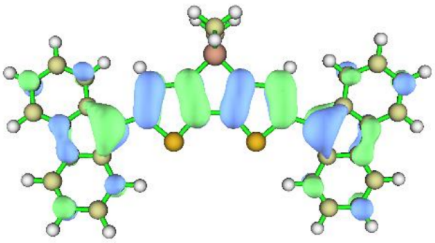
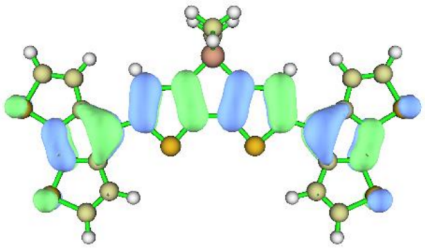
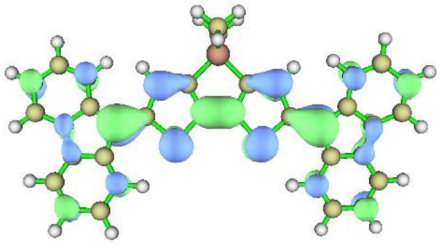
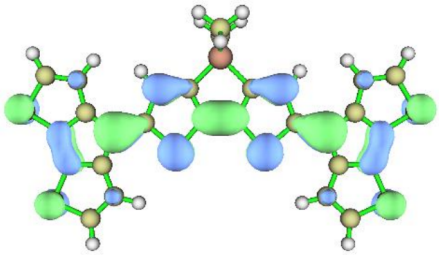
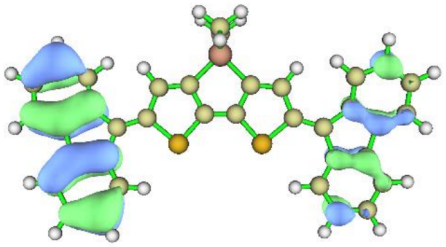
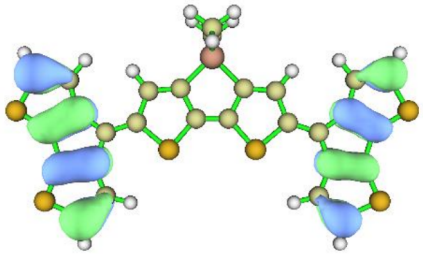
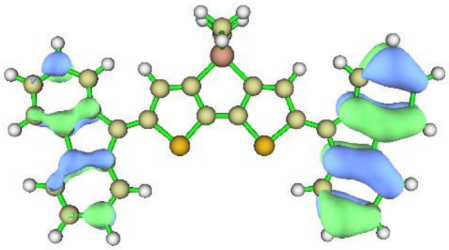
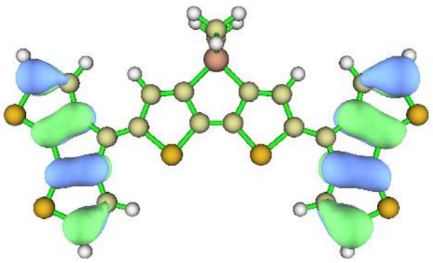
	QP2		QT2
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			
S_1	HOMO → LUMO (100.0 %)	S_1	HOMO-2 → LUMO (76.9 %)
		S_2	HOMO-1 → LUMO (76.9 %)
		S_3	HOMO → LUMO (100 %)
T_1	HOMO → LUMO (96.4 %)	T_1	HOMO → LUMO (96.1 %)

Figure S4: Frontier molecular orbitals with the isovalue of 0.03 a.u. and electronic transitions in the low-lying singlet and triplet states for QP2 and QT2 simulated at the TD-B3LYP/cc-pVDZ level.

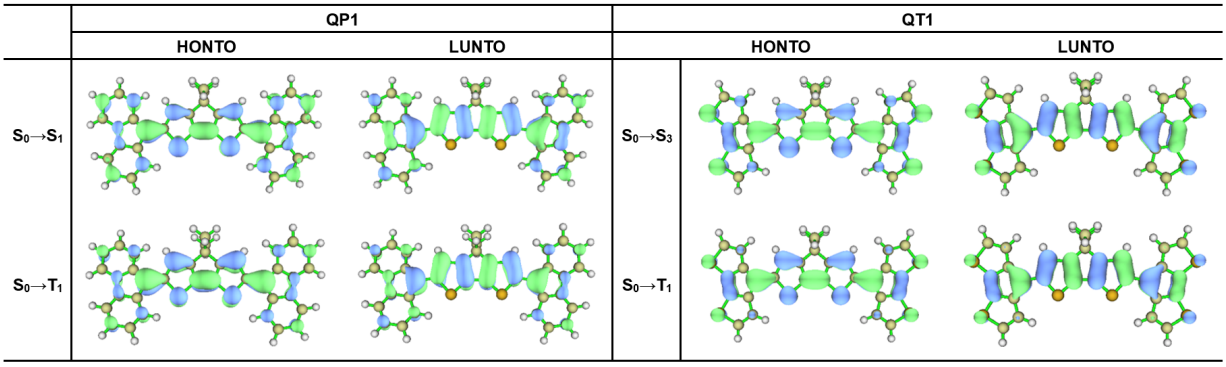


Figure S5: Natural transition orbitals (NTOs) in the bright singlet state and triplet state for QP1 and QT1 simulated at the TD-B3LYP/cc-pVDZ level with the isovalue of 0.03 a.u.

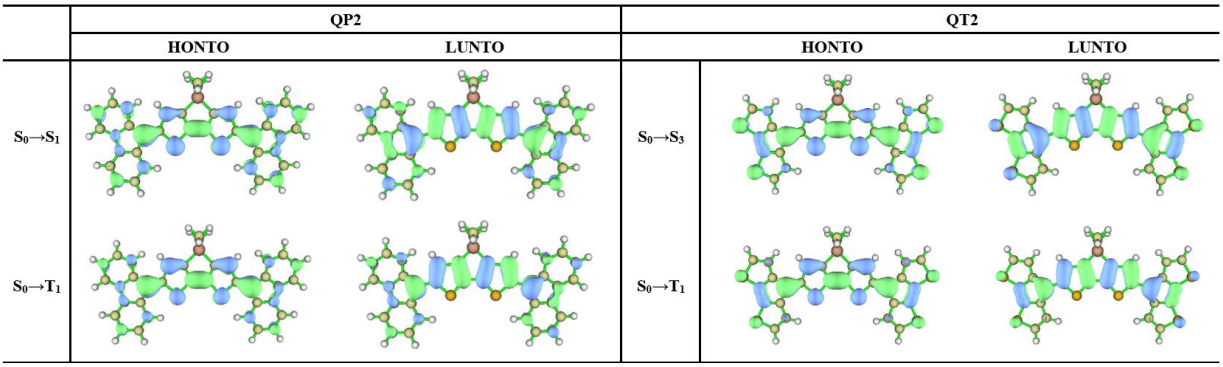


Figure S6: Natural transition orbitals (NTOs) in the bright singlet state and triplet state for QP2 and QT2 with the isovalue of 0.03 a.u. simulated at the TD-B3LYP/cc-pVDZ level.

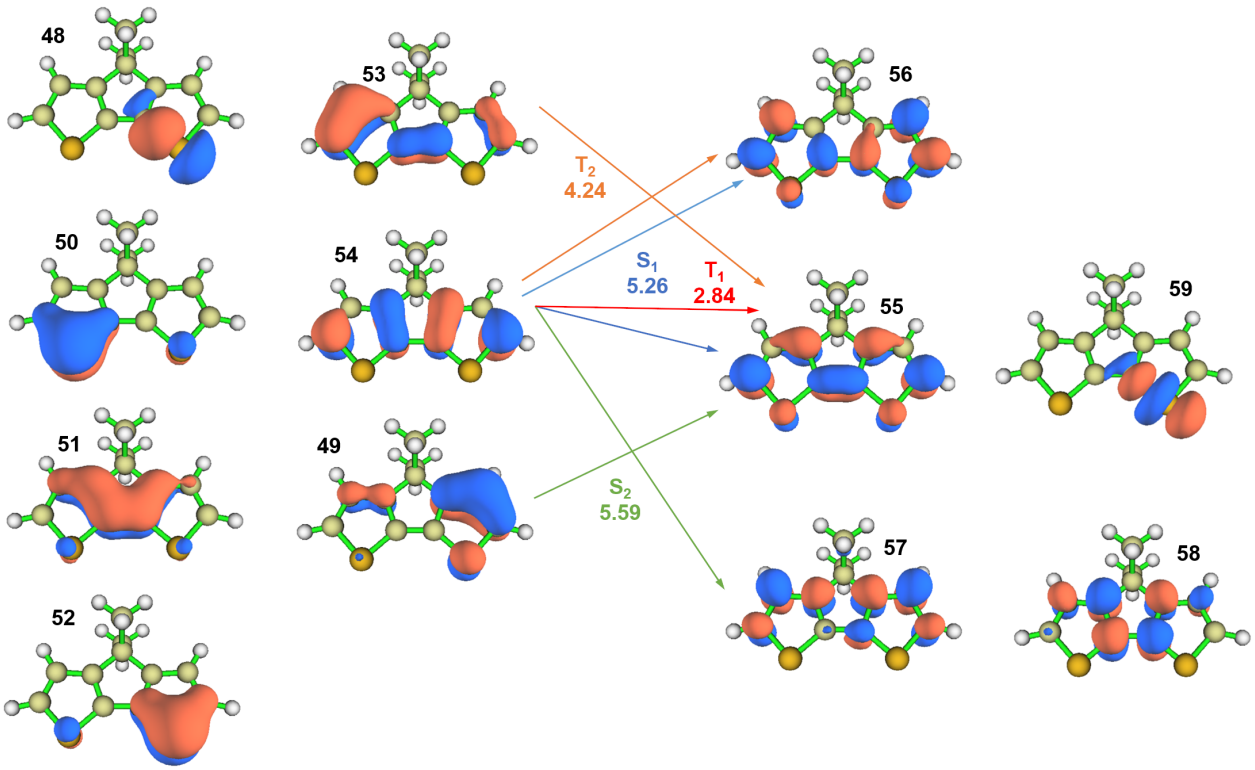


Figure S7: Excitation energies and electronic transitions in low-lying excited states calculated at the MS-CASPT2(14e,12o)/cc-pVDZ level in the DFT optimized structures.

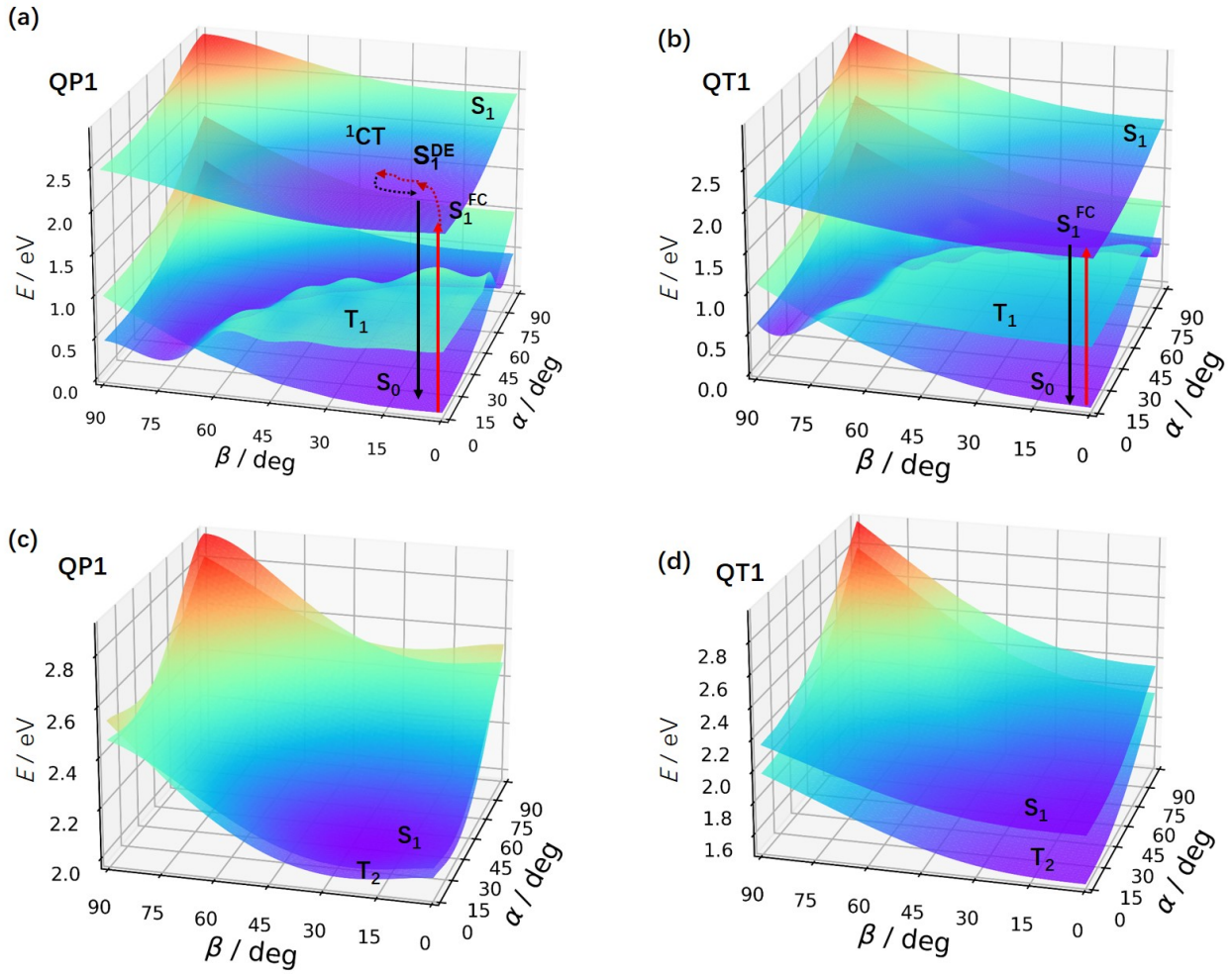


Figure S8: PESs in S_0, S_1, and T_1 states for QP1 (a) and QT1 (b), which show conical intersection between S_0 and T_1 states. PESs in S_1 and T_2 states for QP1 (c) and QT1 (d).

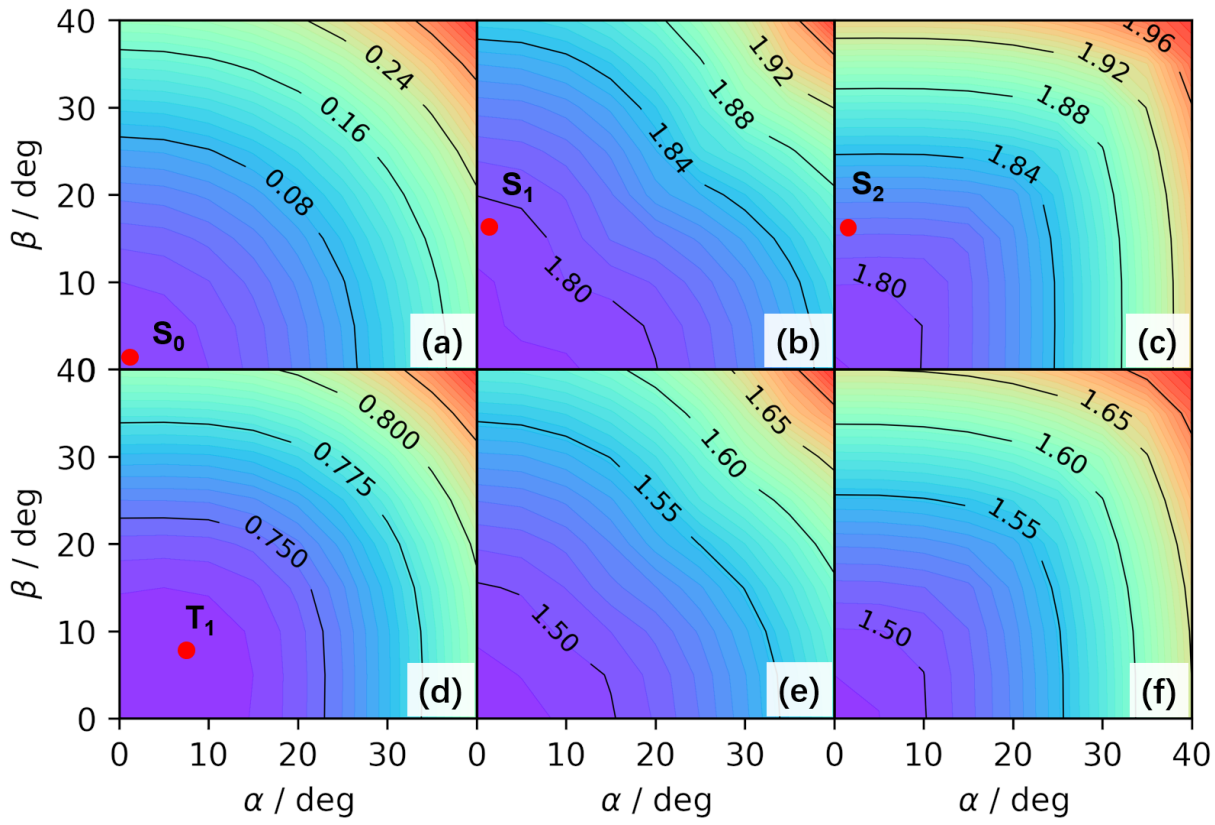


Figure S9: Two-dimensional contour plots of the PESs for QT1 in (a) S_0, (b) S_1, (c) S_2, (d) T_1, (e) T_2, and (f) T_3 states with the optimized structure marked in a red circle in each of the contours.

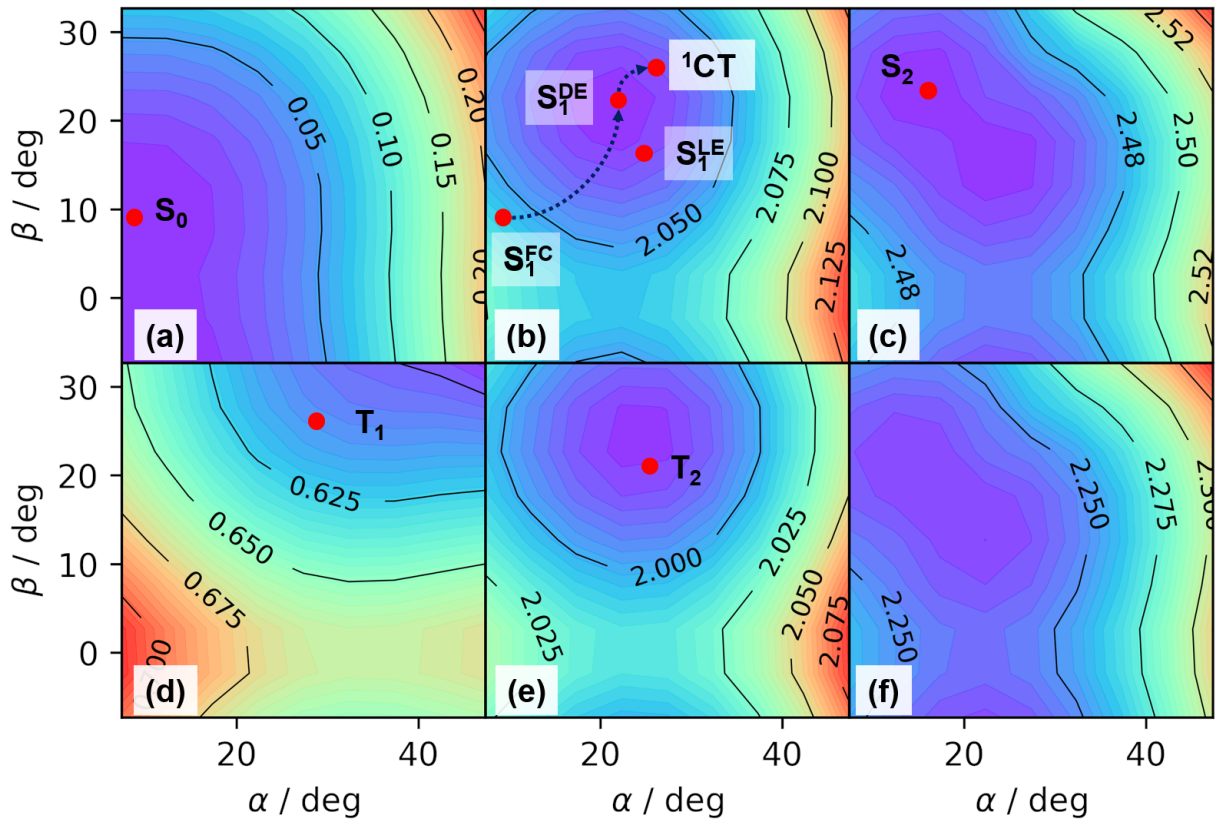


Figure S10: Two-dimensional contour plots of the PESs for QP1 in (a) S_0, (b) S_1, (c) S_2, (d) T_1, (e) T_2, and (f) T_3 state with the optimized structure marked in a red circle in each of the contours.

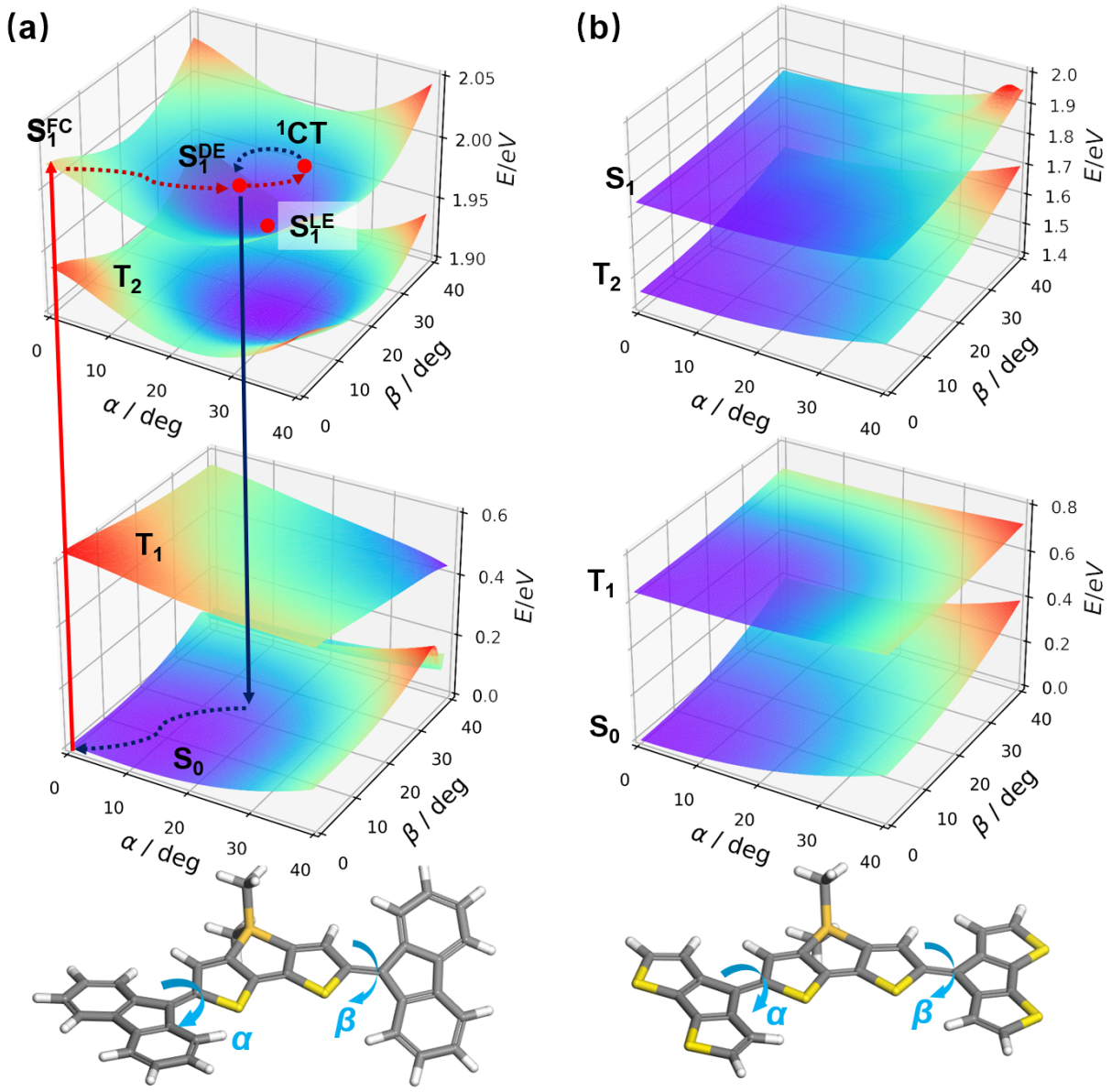


Figure S11: PESs in S_0, S_1, T_1, and T_2 states for QP2 (a) and QT2 (b).

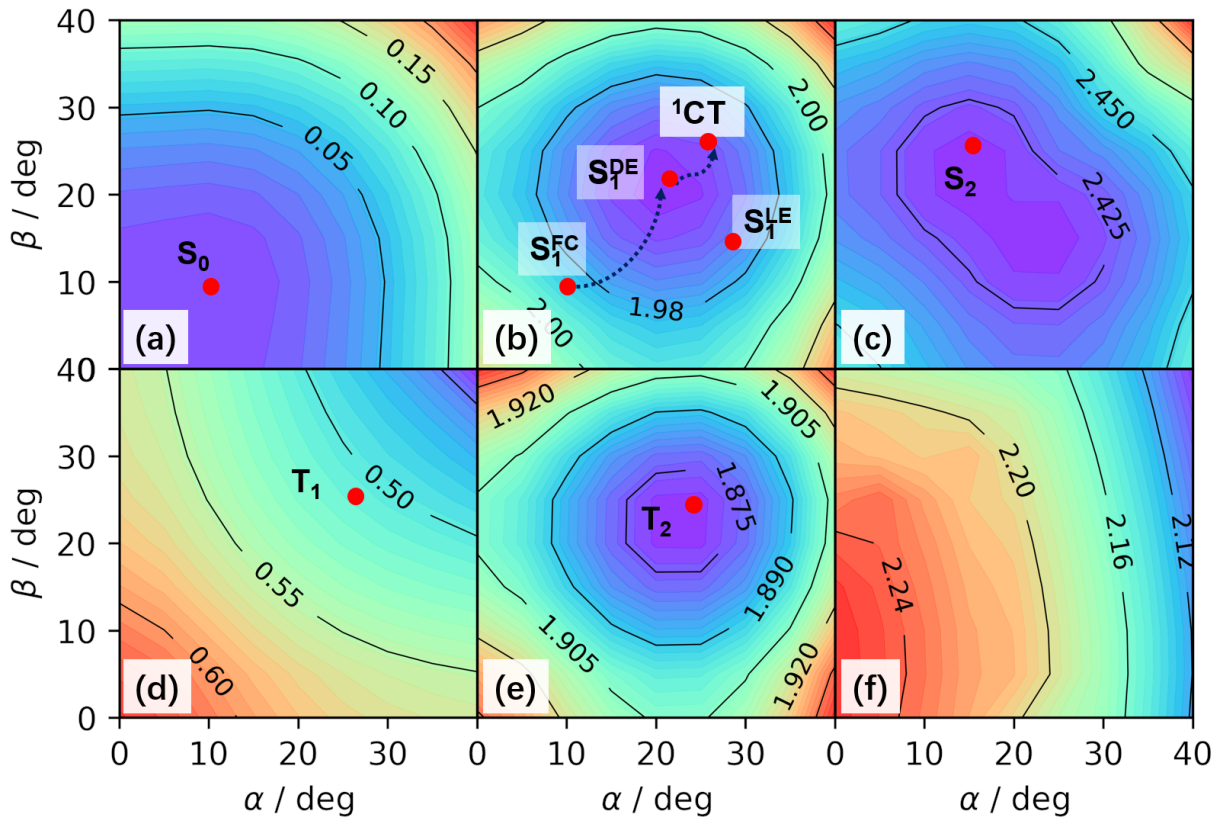


Figure S12: PESs of QP2 in (a) S_0, (b) S_1, (c) S_2, (d) T_1, (e) T_2, and (f) T_3 states with the optimized structure marked in a red circle in each of the contours.

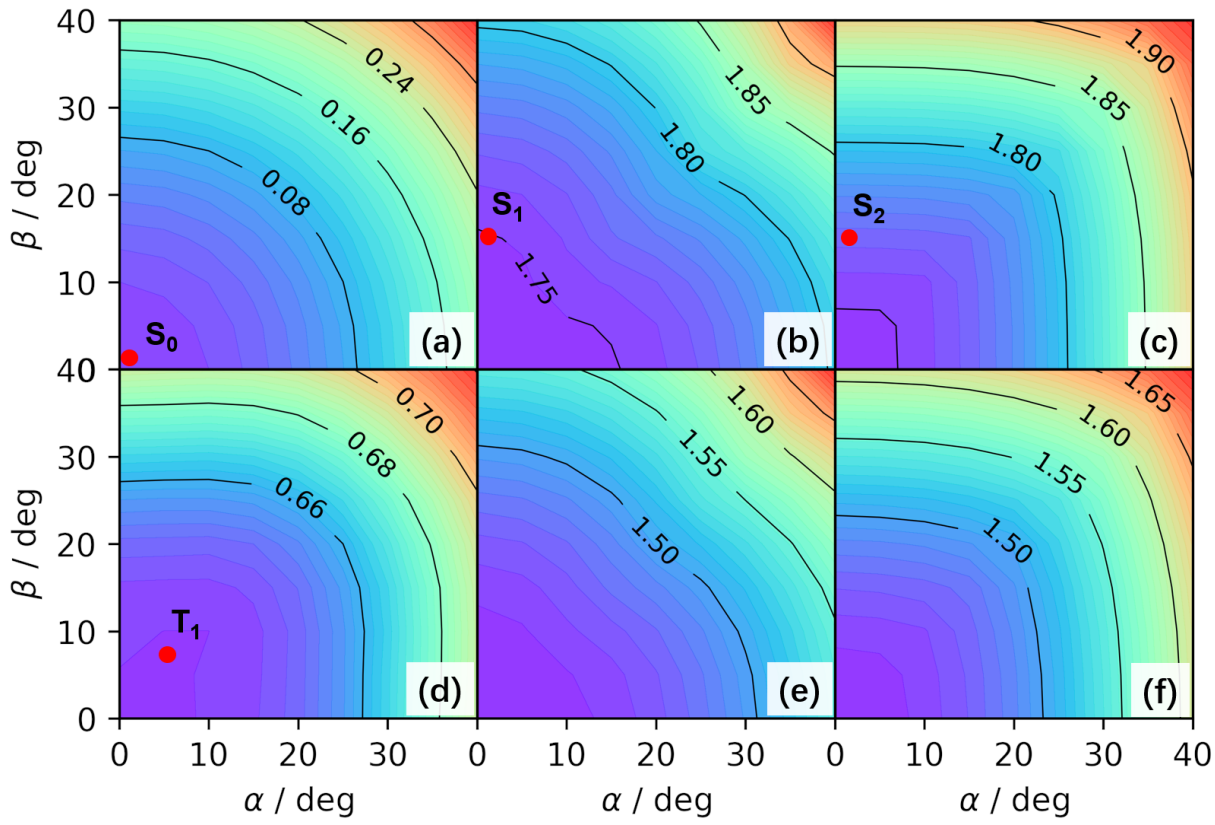


Figure S13: PESs of QT2 in (a) S_0, (b) S_1, (c) S_2, (d) T_1, (e) T_2, and (f) T_3 states calculated at the B3LYP/cc-pVDZ level with the optimized structure marked in a red circle in each of the contours.

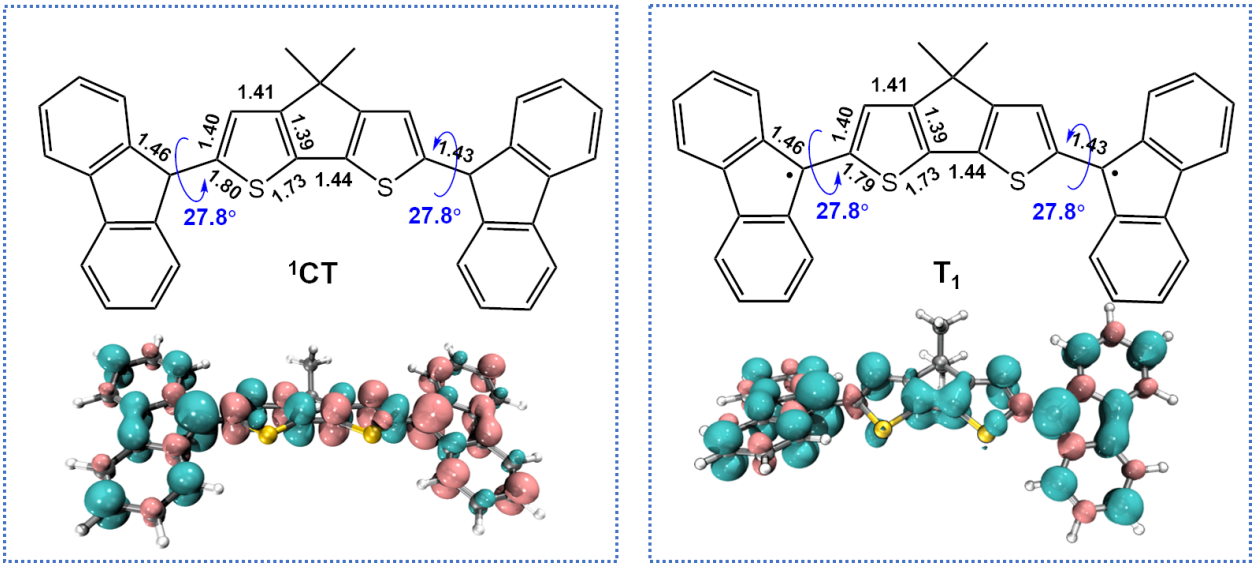


Figure S14: Electron spin density of QP1 in ^{1}CT (left) and T_1 (right) states calculated at the unrestricted B3LYP/cc-pVDZ level. Bond lengths and torsion angles are marked in black and blue respectively. The unpaired electron components are represented in cyan and pink for various spin orientations.

Ultrafast spectra measured in solution and thin film

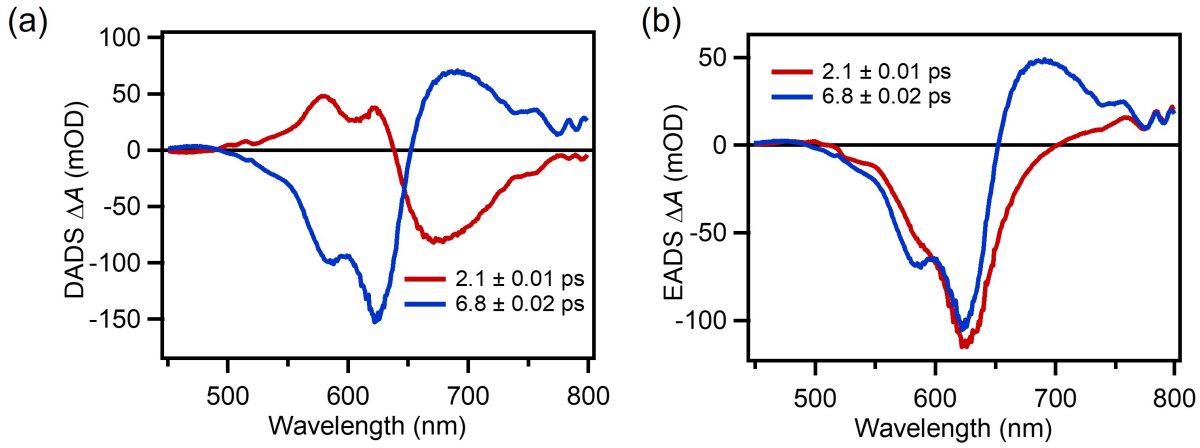
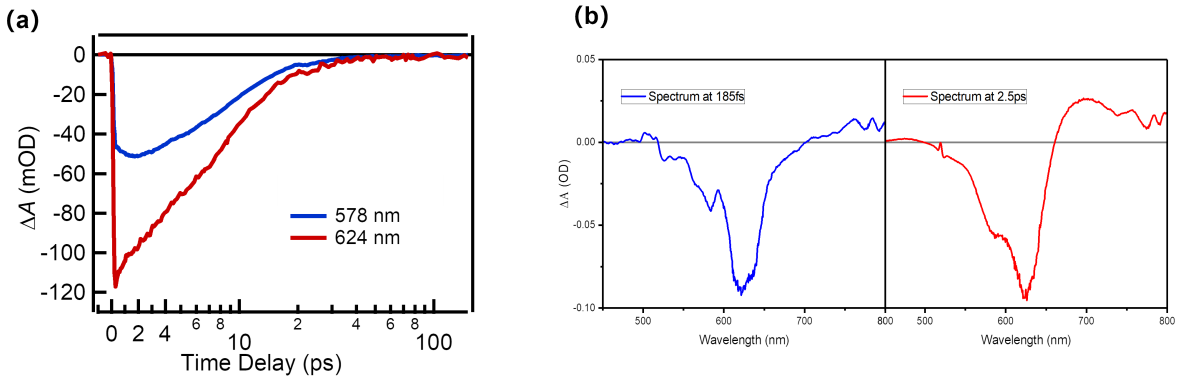


Figure S15: Global analysis of (a) decay-associated difference spectra (DADS) and (b) evolution-associated difference spectra (EADS) of QP1 in dilute DCM solution.



wavelength (nm)	$\Delta A_{0.22\ ps}$ (mOD)	$\Delta A_{2.56\ ps}$ (mOD)	triplet yield (%)
578	-39.46	-49.62	126
624	-110.76	-92.09	83

578 nm: triplet yield = 126%

time delay (ps)	FWHM (nm)	ΔA_{max} (mOD)	area (arb. units)
0.185	58.79	-92.17	4.587
2.500	69.96	-95.35	5.399

triplet yield = 5.399/4.587 = 118%

Figure S16: The triplet yield of QP1 was estimated using two different methods. (a) The ratio method, which was probed by wavelengths of 578 nm and 624 nm. (b) The area approach, which was probed at time delays of 0.185 ps and 2.5 ps.

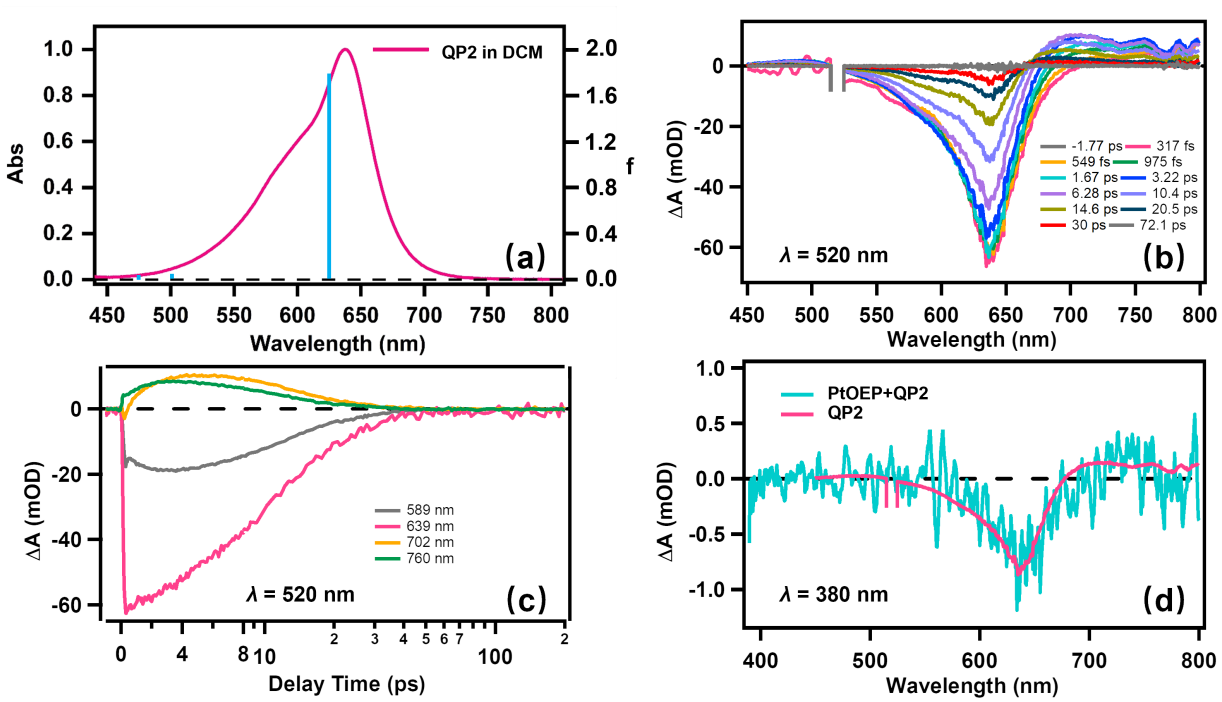


Figure S17: Steady-state absorption spectra with calculated excitation marked in blue bar (a), transient absorption spectrum (b), and kinetic decay measurements excited at 520 nm (c) in dilute DCM solution for QP2. (d) Triplet-sensitization measurements at a time delay of 3.0 ps in magenta for QP2, and 4.2 μs with PtOEP sensitizer in cyan.

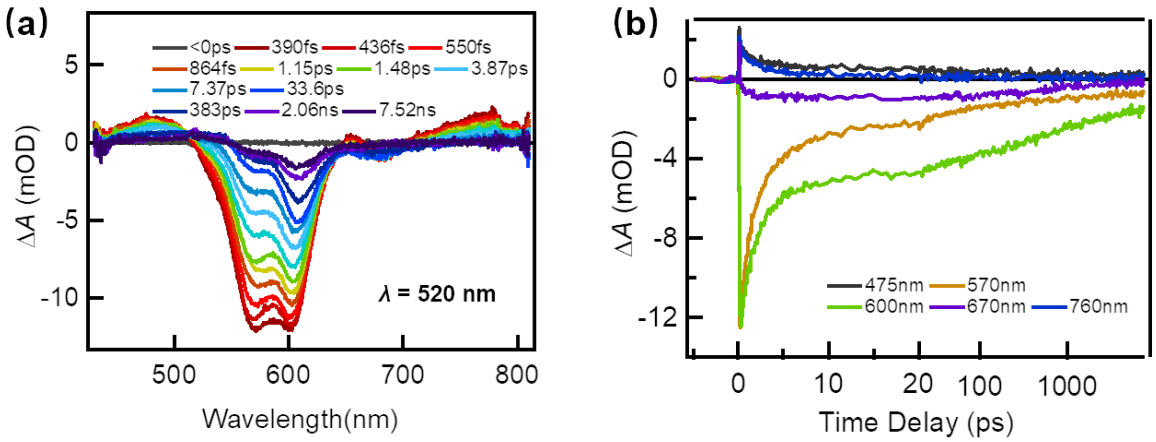


Figure S18: Transient absorption spectrum (a) and kinetic decay measurements excited at 520 nm in a thin film for QP2.

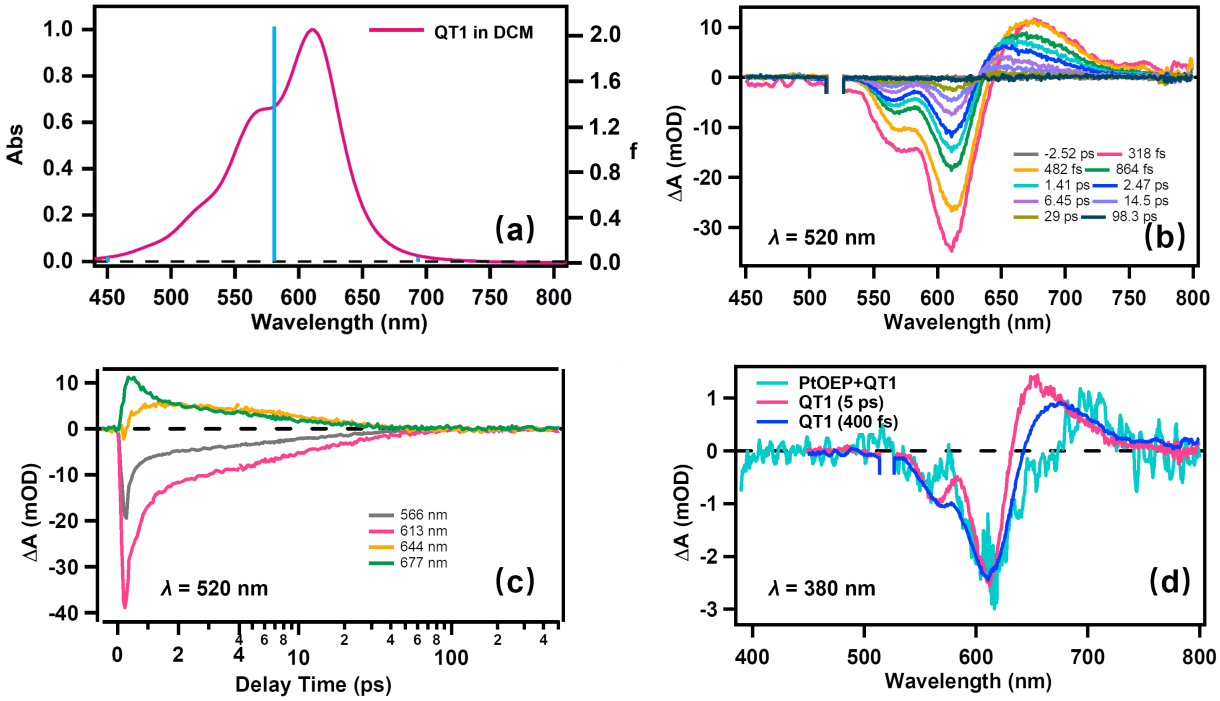


Figure S19: Steady-state absorption spectra with calculated excitation marked in blue bar (a), transient absorption spectrum (b), and kinetic decay measurements excited at 520 nm (c) in dilute DCM solution for QT1. (d) Triplet-sensitization measurements at a time delay of 400 fs in blue and 5 ps in magenta for QT1, and 5 μs with PtOEP sensitizer in cyan.

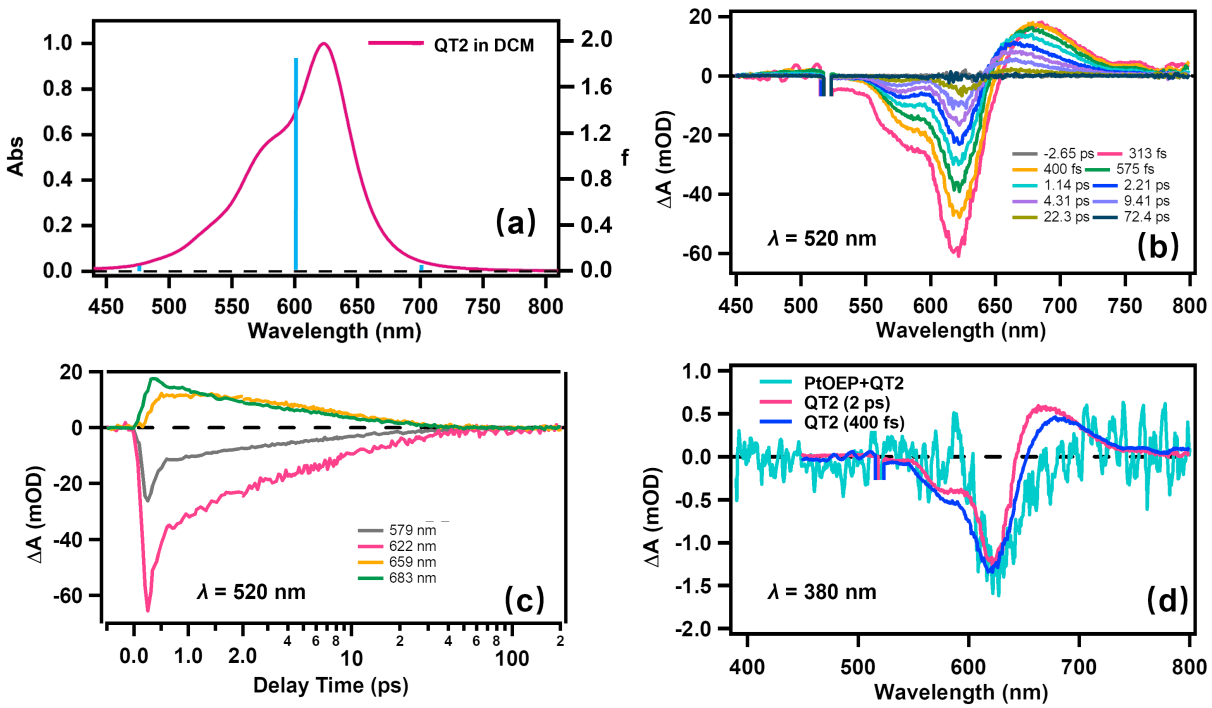


Figure S20: Steady-state absorption spectra with calculated excitation marked in blue bar (a), transient absorption spectrum (b), and kinetic decay measurements excited at 520 nm (c) in dilute DCM solution for QT2. (d) Triplet-sensitization measurements at a time delay of 400 fs in blue and 2 ps in magenta for QT2, and 4.7 μs with PtOEP sensitizer in cyan.

Optimized structures of QT1

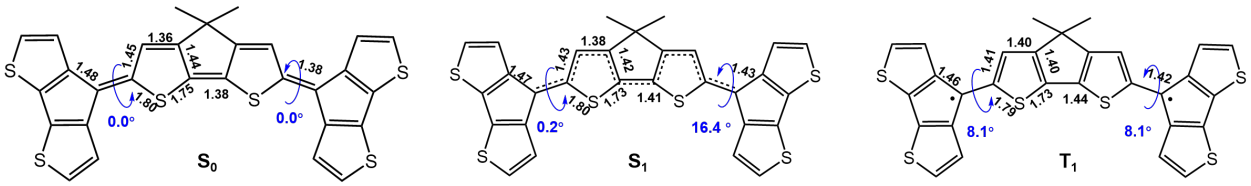


Figure S21: Optimized structures ((bond lengths in black and torsion angles in blue) of QT1 in different states with unpaired-electron components obtained at the B3LYP/cc-pVDZ level.

Optimized coordinates in low-lying excited states of QPs and QTs.

Table S11: Coordinates of the optimized minimum in the S_0 state of QP1 at the B3LYP/cc-pVDZ level.

C	3.22469600	0.12894500	0.02850200
S	1.99781500	-1.20285700	0.01143100
C	0.68991500	-0.05186100	0.00810600
C	1.17235000	1.30134300	0.01410400
C	2.53298600	1.40067400	0.02604800
C	-0.68994600	-0.05183400	-0.00810600
S	-1.99788900	-1.20278000	-0.01144400
C	-3.22472000	0.12906600	-0.02853200
C	-2.53296300	1.40077100	-0.02601000
C	-1.17233100	1.30138700	-0.01406500
C	4.58613400	-0.11361700	0.03266100
C	-4.58615500	-0.11351700	-0.03269500
C	5.66170100	0.89409000	0.19989900
C	6.91867200	0.24163600	0.05645200
C	6.67793900	-1.18192600	-0.17479100
C	5.27290600	-1.40638100	-0.16919400
C	-5.27281200	-1.40633200	0.16916600
C	-6.67786100	-1.18200400	0.17480900
C	-6.91872700	0.24153300	-0.05644500
C	-5.66181700	0.89410000	-0.19994900
C	0.00002800	2.28487000	0.00004300
C	0.01397400	3.16360900	-1.26858500
C	-0.01388600	3.16355100	1.26871200
H	3.07164000	2.34178700	-0.01330400
H	-3.07157200	2.34190200	0.01339400
H	0.02367800	2.54776800	-2.18026600
H	0.90567100	3.81067000	-1.27931800
H	-0.02361300	2.54766800	2.18036400
H	-0.90555900	3.81064400	1.27947600
H	-0.87727900	3.81065200	-1.29820800
H	0.87739100	3.81055900	1.29836600
C	4.79663000	-2.71077300	-0.37336900
C	5.70567700	-3.75660400	-0.56844300
C	7.08648000	-3.52240900	-0.56906600
C	7.57883500	-2.22785000	-0.37387800
C	8.11961700	0.94307400	0.16838500
C	8.08625500	2.31366900	0.44192400
C	6.85765500	2.96217500	0.61903900
C	5.65059400	2.26358200	0.50675000
C	-7.57865100	-2.22801200	0.37392900
C	-7.08616700	-3.52252400	0.56910700
C	-5.70534000	-3.75659000	0.56843900
C	-4.79640000	-2.71067300	0.37333100
C	-5.65086600	2.26358300	-0.50686600
C	-6.85799900	2.96205300	-0.61913300
C	-8.08652900	2.31343800	-0.44194000
C	-8.11974400	0.94285000	-0.16835600
H	3.73242400	-2.93901300	-0.38928400
H	5.32738600	-4.76934200	-0.72315900
H	7.77962900	-4.35211700	-0.72372000
H	8.65499200	-2.04052900	-0.37824700
H	9.07526100	0.42672000	0.05282000
H	9.01808200	2.87601200	0.53201100
H	6.83653900	4.02806900	0.85654400
H	4.72453200	2.80362300	0.69262200
H	-8.65482700	-2.04079300	0.37832900
H	-7.77923200	-4.35229700	0.72378700
H	-5.32694800	-4.76929100	0.72314900
H	-3.73216600	-2.93880000	0.38921500
H	-4.72487800	2.80371400	-0.69281400
H	-6.83699800	4.02793800	-0.85668600
H	-9.01841500	2.87568600	-0.53201600
H	-9.07533300	0.42640500	-0.05274500

Table S12: Coordinates of the optimized minimum in the S_1^{LE} state of QP1 at the B3LYP/cc-pVDZ level.

C	-3.24610	-0.13760	-0.00800
S	-2.01340	1.17910	-0.08800
C	-0.71920	0.02900	-0.01170
C	-1.19460	-1.30070	0.06780
C	-2.57470	-1.39530	0.07090
C	0.69290	0.01850	-0.02500
S	2.01300	1.15540	-0.08430
C	3.21200	-0.16740	0.04230
C	2.54970	-1.40930	0.09850
C	1.15440	-1.30460	0.05710
C	-4.62180	0.12630	-0.02020
C	4.61800	0.10060	0.03720
C	-5.68690	-0.82380	0.33750
C	-6.95050	-0.18990	0.14100
C	-6.70850	1.17240	-0.32610
C	-5.29730	1.36950	-0.41000
C	5.29860	1.29470	0.46730
C	6.74990	1.11390	0.30020
C	6.96360	-0.16040	-0.22890
C	5.64780	-0.80090	-0.40250
C	-0.02090	-2.28250	0.11580
C	-0.02580	-3.22760	-1.10450
C	-0.01610	-3.09370	1.42850
H	-3.12100	-2.33430	0.06770
H	3.09040	-2.34450	0.22880
H	-0.03090	-2.65950	-2.04670
H	-0.91660	-3.87630	-1.08790
H	-0.01520	-2.42950	2.30570
H	0.87640	-3.73820	1.48220
H	0.86650	-3.87450	-1.09530
H	-0.90660	-3.74040	1.48620
C	-4.81420	2.61050	-0.86140
C	-5.71720	3.62410	-1.19540
C	-7.10130	3.42160	-1.09700
C	-7.60170	2.18810	-0.66560
C	-8.14480	-0.85660	0.41460
C	-8.10030	-2.16650	0.90380
C	-6.86490	-2.78830	1.13480
C	-5.66320	-2.12730	0.86350
C	7.67170	2.14390	0.66190
C	7.19090	3.31870	1.18150
C	5.77940	3.48900	1.36060
C	4.85180	2.51190	1.01560
C	5.61880	-2.08550	-0.98170
C	6.81130	-2.70330	-1.33620
C	8.09290	-2.09150	-1.13730
C	8.16850	-0.83310	-0.59680
H	-3.74750	2.80200	-0.97100
H	-5.33440	4.58670	-1.54190
H	-7.78980	4.22670	-1.36300
H	-8.67980	2.02370	-0.59900
H	-9.10510	-0.35940	0.25790
H	-9.02820	-2.70020	1.12080
H	-6.83700	-3.80180	1.54160
H	-4.72580	-2.62940	1.09740
H	8.74360	1.98680	0.52410
H	7.86840	4.12530	1.46500
H	5.41890	4.42720	1.78980
H	3.79160	2.69570	1.18650
H	4.67370	-2.59030	-1.17610
H	6.77510	-3.69700	-1.78990
H	8.99500	-2.63190	-1.42730
H	9.13230	-0.34090	-0.45110

Table S13: Coordinates of the optimized minimum in S_1^{DE} state of QP1 at the B3LYP/cc-pVDZ level.

C	3.22284400	0.15160900	-0.04049800
S	2.00162200	-1.17349900	-0.02499400
C	0.70606900	-0.01945100	-0.00225800
C	1.17459000	1.31474200	-0.00480300
C	2.56043000	1.41024500	-0.02634000
C	-0.70606900	-0.01945200	0.00222600
S	-2.00162000	-1.17350200	0.02495500
C	-3.22284400	0.15160400	0.04048200
C	-2.56043200	1.41024100	0.02631600
C	-1.17459200	1.31474000	0.00477400
C	4.60770300	-0.11721600	-0.04185400
C	-4.60770200	-0.11722200	0.04185300
C	5.65461800	0.80739400	0.39270800
C	6.92623000	0.17950000	0.20971700
C	6.69490900	-1.15687100	-0.33453800
C	5.28354800	-1.33663500	-0.47849200
C	-5.28354400	-1.33664100	0.47849500
C	-6.69490600	-1.15687500	0.33455700
C	-6.92623200	0.17949800	-0.20969000
C	-5.65462100	0.80739100	-0.39269300
C	-0.00000200	2.29680400	-0.00001600
C	-0.00595500	3.17560000	-1.26879300
C	0.00595100	3.17560400	1.26875800
H	3.11191700	2.34438400	-0.10172200
H	-3.11192100	2.34437900	0.10170200
H	-0.01163400	2.55905000	-2.18007500
H	0.88600100	3.82230500	-1.29473800
H	0.01163000	2.55905700	2.18004200
H	-0.88600700	3.82230800	1.29470100
H	-0.89705400	3.82381200	-1.28440900
H	0.89704900	3.82381700	1.28437200
C	4.80165700	-2.54133100	-1.02376600
C	5.70567200	-3.54634400	-1.38024900
C	7.08677100	-3.36591900	-1.21669700
C	7.58660300	-2.16290500	-0.69835900
C	8.10545700	0.83404100	0.55796600
C	8.03719300	2.12188200	1.10755100
C	6.79376800	2.73394700	1.32331500
C	5.60416700	2.08603900	0.97826000
C	-7.58659800	-2.16290900	0.69838500
C	-7.08676200	-3.36592500	1.21671300
C	-5.70566100	-3.54635300	1.38024900
C	-4.80164900	-2.54133900	1.02376000
C	-5.60417500	2.08603900	-0.97824000
C	-6.79377800	2.73395000	-1.32327900
C	-8.03720100	2.12188600	-1.10750400
C	-8.10546100	0.83404300	-0.55792300
H	3.73652800	-2.70314500	-1.19062600
H	5.32775400	-4.48168100	-1.79908100
H	7.77679900	-4.16277900	-1.50286500
H	8.66386000	-2.01861600	-0.58640200
H	9.07392000	0.34907400	0.41398100
H	8.95571500	2.64497500	1.38265200
H	6.75121100	3.72740500	1.77557800
H	4.65312300	2.57100600	1.19637700
H	-8.66385600	-2.01861800	0.58644100
H	-7.77678700	-4.16278500	1.50288600
H	-5.32773900	-4.48169200	1.79907300
H	-3.73651800	-2.70315700	1.19060600
H	-4.65313200	2.57100500	-1.19636500
H	-6.75122400	3.72741000	-1.77553800
H	-8.95572600	2.64498200	-1.38259200
H	-9.07392300	0.34907700	-0.41392900

Table S14: Coordinates of the optimized minimum in the ^{1}CT state of QP1 at the B3LYP/cc-pVDZ level.

S	2.01687100	1.08561500	-0.43764600
C	0.72063100	0.01312600	-0.02515300
C	1.17394000	-1.21057200	0.46138600
C	2.57890400	-1.29885600	0.50478000
C	-0.72074900	0.01289100	-0.02615600
S	-2.01692900	1.08615600	-0.43704000
C	-3.22622100	-0.13743300	0.05541300
C	-2.57911400	-1.29974200	0.50203500
C	-1.17416500	-1.21129600	0.45922800
C	4.63155200	0.11331900	-0.04349000
C	-4.63149400	0.11315400	-0.04430300
C	5.66586600	-0.90728300	-0.21039100
C	6.94101100	-0.26569000	-0.23311800
C	6.72410600	1.17544900	-0.08770700
C	5.31783800	1.40146500	0.01868000
C	-5.31767300	1.40103500	0.02060900
C	-6.72397400	1.17535900	-0.08579700
C	-6.94096400	-0.26543200	-0.23523300
C	-5.66586200	-0.90712100	-0.21325300
C	-0.00015500	-2.12146100	0.82847000
C	-0.00152800	-2.46057900	2.33450900
C	0.00107100	-3.41336500	-0.01625800
H	3.13248400	-2.14809900	0.90025900
H	-3.13281200	-2.14977600	0.89585000
H	-0.00199700	-1.54705900	2.94784100
H	0.88912900	-3.05351800	2.59835800
H	0.00245900	-3.18483500	-1.09265600
H	-0.88998100	-4.02224900	0.20697500
H	-0.89273700	-3.05340100	2.59679600
H	0.89166700	-4.02207300	0.20929300
C	4.84451900	2.71167200	0.20257600
C	5.75740900	3.76996800	0.24889900
C	7.13503400	3.53945300	0.12702400
C	7.62500100	2.23625100	-0.03569300
C	8.11014400	-1.00467600	-0.39844600
C	8.02223000	-2.39489900	-0.55428700
C	6.77246000	-3.03048900	-0.56242600
C	5.59280900	-2.29737200	-0.39860700
C	-7.62487300	2.23581400	-0.03038100
C	-7.13483700	3.53869600	0.13536800
C	-5.75712300	3.76884500	0.25721300
C	-4.84419300	2.71073800	0.20793000
C	-5.59272700	-2.29684400	-0.40359100
C	-6.77239700	-3.02952100	-0.56914300
C	-8.02213800	-2.39380100	-0.56084000
C	-8.11015400	-1.00388600	-0.40258000
H	3.78044000	2.91619100	0.32322300
H	5.38985600	4.78896500	0.38786600
H	7.83142700	4.37985800	0.16681900
H	8.70000900	2.05876400	-0.11554400
H	9.08412000	-0.51008900	-0.41514000
H	8.93202400	-2.98510900	-0.68352500
H	6.71706800	-4.11169100	-0.70706900
H	4.63176100	-2.80940000	-0.44491300
H	-8.69987500	2.05859200	-0.11078100
H	-7.83131700	4.37890400	0.17784300
H	-5.38951500	4.78740500	0.39909300
H	-3.77999600	2.91493500	0.32856400
H	-4.63166400	-2.80896200	-0.44995000
H	-6.71688400	-4.11049200	-0.71535800
H	-8.93194200	-2.98366000	-0.69167500
H	-9.08404100	-0.50913300	-0.41910800

Table S15: Coordinates of the optimized minimum in the S_2 state of QP1 at the B3LYP/cc-pVDZ level.

C	3.21196200	-0.16738600	0.04234500
S	2.01295300	1.15542700	-0.08437100
C	0.69288900	0.01846700	-0.02494300
C	1.15439400	-1.30460600	0.05723300
C	2.54969800	-1.40925800	0.09862900
C	-0.71920600	0.02896900	-0.01181100
S	-2.01338800	1.17903400	-0.08809100
C	-3.24606000	-0.13772800	-0.00814500
C	-2.57473000	-1.39540100	0.07084600
C	-1.19460700	-1.30079900	0.06779700
C	4.61795500	0.10063500	0.03725200
C	-4.62177200	0.12618100	-0.02037600
C	5.64779900	-0.80078300	-0.40262300
C	6.96364300	-0.16034500	-0.22899600
C	6.74988200	1.11395800	0.30025200
C	5.29858700	1.29466500	0.46739600
C	-5.29730300	1.36943600	-0.41023300
C	-6.70849900	1.17242800	-0.32607200
C	-6.95049500	-0.18980500	0.14118600
C	-5.68689600	-0.82380300	0.33753600
C	-0.02081300	-2.28254400	0.11576200
C	-0.01617500	-3.09385700	1.42841400
C	-0.02567200	-3.22759700	-1.10456200
H	3.09053000	-2.34440000	0.22904300
H	-3.12102300	-2.33437200	0.06768900
H	-0.01534000	-2.42970700	2.30566200
H	0.87635500	-3.73825700	1.48212000
H	-0.03075300	-2.65935200	-2.04678200
H	-0.91639900	-3.87628500	-1.08800100
H	-0.90659800	-3.74058700	1.48597300
H	0.86672700	-3.87435800	-1.09536100
C	4.85173800	2.51175500	1.01594400
C	5.77940200	3.48884800	1.36104600
C	7.19086000	3.31860100	1.18196800
C	7.67173300	2.14388700	0.66208300
C	8.16851600	-0.83300200	-0.59699200
C	8.09285300	-2.09133300	-1.13759300
C	6.81123900	-2.70318700	-1.33645400
C	5.61872500	-2.08537900	-0.98185600
C	-7.60158200	2.18816300	-0.66552900
C	-7.10120000	3.42157100	-1.09715700
C	-5.71710300	3.62396600	-1.19586400
C	-4.81413400	2.61032000	-0.86192100
C	-5.66326900	-2.12731000	0.86353000
C	-6.86499500	-2.78810700	1.13509600
C	-8.10039800	-2.16620900	0.90427600
C	-8.14483200	-0.85634500	0.41498400
H	3.79154300	2.69559600	1.18679600
H	5.41883300	4.42691400	1.79047900
H	7.86841100	4.12506300	1.46560200
H	8.74356500	1.98688800	0.52431700
H	9.13234600	-0.34079800	-0.45134400
H	8.99492500	-2.63174400	-1.42773100
H	6.77503300	-3.69685100	-1.79019900
H	4.67367800	-2.59015900	-1.17622000
H	-8.67972500	2.02394300	-0.59874700
H	-7.78968900	4.22664000	-1.36322600
H	-5.33429400	4.58645300	-1.54266500
H	-3.74742600	2.80168800	-0.97172200
H	-4.72596800	-2.62953500	1.09733600
H	-6.83717400	-3.80163000	1.54186100
H	-9.02829700	-2.69980200	1.12139900
H	-9.10510200	-0.35912500	0.25845200

Table S16: Coordinates of the optimized minimum in the T_1 state of QP1 at the B3LYP/cc-pVDZ level.

C	3.22430700	0.15176600	-0.03896800
S	2.01374100	-1.16605800	-0.02665700
C	0.71936400	-0.01758400	-0.00493000
C	1.17391900	1.30008500	-0.00549300
C	2.57684100	1.39730600	-0.02204200
C	-0.71936600	-0.01759100	0.00464000
S	-2.01373200	-1.16607800	0.02627900
C	-3.22430700	0.15173600	0.03881300
C	-2.57685500	1.39728200	0.02182700
C	-1.17393300	1.30007400	0.00522900
C	4.62755000	-0.12027300	-0.04452500
C	-4.62754800	-0.12031100	0.04452000
C	5.66369500	0.76329100	0.48383200
C	6.93828800	0.15621800	0.26505800
C	6.71659600	-1.12824600	-0.40123800
C	5.30831000	-1.29430200	-0.57996800
C	-5.30824800	-1.29436000	0.57999400
C	-6.71655400	-1.12830200	0.40141600
C	-6.93831900	0.15618700	-0.26480700
C	-5.66375000	0.76327300	-0.48368900
C	-0.00001100	2.28216700	-0.00014400
C	-0.00535000	3.16206100	-1.26851600
C	0.00531900	3.16208300	1.26821200
H	3.13045400	2.33238200	-0.07924000
H	-3.13047400	2.33235200	0.07906700
H	-0.01125600	2.54581700	-2.18007500
H	0.88651900	3.80887000	-1.29446200
H	0.01123200	2.54585500	2.17978200
H	-0.88655600	3.80888400	1.29414600
H	-0.89539000	3.81174400	-1.28421100
H	0.89535300	3.81177400	1.28389500
C	4.83011400	-2.44199300	-1.23627600
C	5.73866700	-3.41097200	-1.67247200
C	7.11745400	-3.24676700	-1.47630600
C	7.61272200	-2.09751100	-0.84417400
C	8.10904800	0.78012900	0.68883100
C	8.02472600	2.01503900	1.34711500
C	6.77628800	2.60473700	1.59284900
C	5.59473600	1.98593900	1.17328000
C	-7.61263100	-2.09758600	0.84440900
C	-7.11729400	-3.24686400	1.47644600
C	-5.73848700	-3.41107300	1.67246400
C	-4.82998200	-2.44207400	1.23621000
C	-5.59486300	1.98595100	-1.17308900
C	-6.77646000	2.60476400	-1.59251100
C	-8.02487200	2.01505200	-1.34667400
C	-8.10912400	0.78011400	-0.68843200
H	3.76531800	-2.58314400	-1.42334800
H	5.36721900	-4.30452300	-2.17875400
H	7.81060300	-4.01501600	-1.82577800
H	8.68857300	-1.96598100	-0.70703100
H	9.08200100	0.31278500	0.51988000
H	8.93623900	2.51428700	1.68275900
H	6.72384200	3.55605900	2.12688500
H	4.63489200	2.44561600	1.40871000
H	-8.68849700	-1.96605400	0.70738300
H	-7.81040500	-4.01512800	1.82596200
H	-5.36698400	-4.30464200	2.17867300
H	-3.76516600	-2.58323100	1.42316700
H	-4.63504400	2.44564100	-1.40859600
H	-6.72407200	3.55611000	-2.12651000
H	-8.93642000	2.51431200	-1.68220200
H	-9.08205900	0.31276100	-0.51940000

Table S17: Coordinates of the optimized minimum in the T_2 state of QP1 at the B3LYP/cc-pVDZ level.

C	-3.24155700	-0.13634200	-0.00918800
S	-2.01602900	1.18010000	-0.07202700
C	-0.71965400	0.02931100	0.00530600
C	-1.18965500	-1.29342100	0.07619400
C	-2.57797000	-1.38957700	0.06949700
C	0.70209100	0.01856200	-0.00218800
S	2.01458200	1.15519000	-0.05410300
C	3.21731200	-0.16736100	0.05442700
C	2.55876900	-1.40531000	0.10390400
C	1.15997400	-1.30261700	0.07068100
C	-4.62650300	0.12920000	-0.02880300
C	4.62659100	0.10151300	0.04207600
C	-5.68617400	-0.80383800	0.37543200
C	-6.95202700	-0.17915000	0.16180600
C	-6.71303100	1.16146100	-0.36711900
C	-5.30178100	1.35261800	-0.47013100
C	5.31123300	1.26576800	0.52291700
C	6.76447300	1.09833000	0.32659400
C	6.96947100	-0.14838000	-0.26702900
C	5.64656800	-0.77328500	-0.45748800
C	-0.01815200	-2.27805200	0.12481800
C	-0.02496500	-3.22235200	-1.09598600
C	-0.01947500	-3.09087800	1.43671400
H	-3.12584900	-2.32808700	0.05754600
H	3.10187700	-2.34173100	0.22158000
H	-0.02425700	-2.65333100	-2.03779000
H	-0.91954000	-3.86587200	-1.08274400
H	-0.01710600	-2.42739600	2.31449900
H	0.86962700	-3.74011700	1.49165800
H	0.86312700	-3.87524300	-1.08503400
H	-0.91317500	-3.73332600	1.49237200
C	-4.81851100	2.56936200	-0.98320100
C	-5.72206400	3.56845600	-1.35711600
C	-7.10585500	3.37399300	-1.23814300
C	-7.60617400	2.16287800	-0.74649000
C	-8.14261600	-0.83502400	0.47449100
C	-8.09114300	-2.12297300	1.01922700
C	-6.85297400	-2.73374300	1.26545200
C	-5.65446600	-2.08397300	0.95555400
C	7.68282100	2.11672400	0.73035600
C	7.19885900	3.25718700	1.31617200
C	5.78469400	3.41054000	1.52659800
C	4.86139300	2.44998800	1.14505900
C	5.59476100	-2.02543500	-1.10667300
C	6.77377100	-2.63287800	-1.50764600
C	8.06583200	-2.04093400	-1.28943100
C	8.16279600	-0.81402800	-0.68589100
H	-3.75136200	2.74900200	-1.11015600
H	-5.34057100	4.51286800	-1.75191600
H	-7.79471000	4.16762000	-1.53592300
H	-8.68428400	2.00488700	-0.66497300
H	-9.10541200	-0.34682500	0.30526000
H	-9.01635400	-2.64789400	1.26702200
H	-6.82095100	-3.72927800	1.71427900
H	-4.71210300	-2.57248000	1.19933100
H	8.75427100	1.97750600	0.57206600
H	7.87397900	4.05339200	1.63308400
H	5.42736900	4.32184300	2.01238100
H	3.80158800	2.61203500	1.33993100
H	4.63972600	-2.50599400	-1.31534100
H	6.72432600	-3.59883100	-2.01639500
H	8.95858500	-2.57433500	-1.61904200
H	9.13437300	-0.34111500	-0.52812600

Table S18: Coordinates of the optimized minimum in the S_0 state of QP2 at the B3LYP/cc-pVDZ level.

C	3.23765000	0.17457300	0.02386000
S	1.84925900	-0.97100000	0.00710200
C	0.69292000	0.34487400	0.00572900
C	1.34889200	1.63162800	0.00985000
C	2.71344200	1.52275000	0.02137500
C	-0.69292500	0.34487800	-0.00573900
S	-1.84927300	-0.97098800	-0.00710800
C	-3.23765700	0.17459200	-0.02387100
C	-2.71344000	1.52276700	-0.02138300
C	-1.34889000	1.63163700	-0.00986100
C	4.55901300	-0.23860500	0.02381700
C	-4.55901900	-0.23858900	-0.02382200
C	5.75556500	0.62149900	0.18978300
C	6.91768800	-0.18662300	0.03678000
C	6.49443500	-1.56653500	-0.19801300
C	5.07209800	-1.60741200	-0.18433800
C	-5.07208500	-1.60740200	0.18433400
C	-6.49442200	-1.56654600	0.19802200
C	-6.91769600	-0.18663900	-0.03676800
C	-5.75558500	0.62150000	-0.18978300
Si	0.00000500	2.97559100	-0.00000500
C	0.00780800	4.03718500	-1.56104000
C	-0.00778900	4.03718200	1.56103300
H	3.37907300	2.37975500	-0.01807100
H	-3.37906500	2.37977700	0.01806600
H	0.01174100	3.40839700	-2.46501100
H	0.89989300	4.68510600	-1.58686200
H	-0.01173800	3.40839000	2.46500300
H	-0.89986400	4.68511700	1.58685200
H	-0.88296000	4.68655000	-1.59518300
H	0.88298900	4.68653200	1.59518400
C	4.42870500	-2.83801000	-0.38812500
C	5.19325100	-3.99220000	-0.59209600
C	6.59274400	-3.93872300	-0.60135300
C	7.25060300	-2.71963000	-0.40577800
C	8.19929300	0.35401400	0.14514800
C	8.34373500	1.71620000	0.42511200
C	7.20962400	2.51628700	0.61247800
C	5.92219100	1.97929800	0.50390300
C	-7.25057100	-2.71965100	0.40579100
C	-6.59269300	-3.93873500	0.60135900
C	-5.19319900	-3.99219200	0.59209000
C	-4.42867200	-2.83799100	0.38811400
C	-5.92223700	1.97929600	-0.50390500
C	-7.20967900	2.51626500	-0.61246800
C	-8.34377700	1.71616100	-0.42508900
C	-8.19931000	0.35397800	-0.14512500
H	3.34357400	-2.92457500	-0.39583000
H	4.68614000	-4.94700400	-0.74658500
H	7.17146500	-4.85078900	-0.76274800
H	8.34195400	-2.67391000	-0.41658100
H	9.08008700	-0.28030300	0.02220400
H	9.34059500	2.15355900	0.51265200
H	7.32703500	3.57465900	0.85553200
H	5.07364300	2.63214600	0.69801300
H	-8.34192300	-2.67394800	0.41660300
H	-7.17139900	-4.85081000	0.76275900
H	-4.68607200	-4.94698800	0.74657400
H	-3.34353900	-2.92453900	0.39580900
H	-5.07370400	2.63215900	-0.69802500
H	-7.32710900	3.57463400	-0.85552400
H	-9.34064400	2.15350400	-0.51262200
H	-9.08009400	-0.28035300	-0.02217200

Table S19: Coordinates of the optimized minimum in the S_1^{DE} state of QP2 at the B3LYP/cc-pVDZ level.

C	3.23275900	0.20594800	-0.05731300
S	1.84340400	-0.92688600	-0.03377400
C	0.70966200	0.39720000	-0.00884600
C	1.35442000	1.66301100	-0.01842200
C	2.74324000	1.53994700	-0.04505500
C	-0.70966200	0.39720100	0.00886300
S	-1.84340600	-0.92688300	0.03380400
C	-3.23276000	0.20595300	0.05732000
C	-2.74323900	1.53995200	0.04506700
C	-1.35441900	1.66301300	0.01843600
C	4.56988700	-0.24611900	-0.06732400
C	-4.56988900	-0.24611400	0.06732100
C	5.73506700	0.52964600	0.35721000
C	6.90927900	-0.26303600	0.16400000
C	6.49576900	-1.55690000	-0.37586300
C	5.07177600	-1.54553900	-0.50621500
C	-5.07177800	-1.54553300	0.50621300
C	-6.49577100	-1.55689600	0.37585400
C	-6.90927900	-0.26303600	-0.16401800
C	-5.73506600	0.52964700	-0.35722500
Si	0.00000200	3.00183700	0.00000900
C	-0.02446100	4.06733200	-1.55948500
C	0.02446700	4.06732300	1.55950900
H	3.42370100	2.38526800	-0.12489700
H	-3.42369800	2.38527400	0.12490600
H	-0.03925200	3.43999800	-2.46439900
H	0.86702300	4.71531400	-1.60290900
H	0.03924400	3.43998300	2.46441900
H	-0.86700900	4.71531700	1.60293200
H	-0.91576900	4.71687400	-1.57421500
H	0.91578400	4.71685300	1.57425000
C	4.42621400	-2.67550300	-1.04177600
C	5.18322500	-3.79362400	-1.40414900
C	6.57763100	-3.79988800	-1.25522000
C	7.24026100	-2.67422300	-0.74527800
C	8.16855500	0.22764400	0.50107400
C	8.27801500	1.51303100	1.04977000
C	7.12976500	2.28611300	1.27573000
C	5.86106200	1.80328900	0.94198000
C	-7.24026200	-2.67421900	0.74527000
C	-6.57763300	-3.79988100	1.25522000
C	-5.18322800	-3.79361500	1.40415500
C	-4.42621700	-2.67549400	1.04178200
C	-5.86106100	1.80328600	-0.94200500
C	-7.12976300	2.28610600	-1.27576500
C	-8.27801200	1.51302400	-1.04980600
C	-8.16855400	0.22764000	-0.50110100
H	3.34693100	-2.69290200	-1.19496200
H	4.67876700	-4.67082500	-1.81540700
H	7.15132400	-4.68278300	-1.54576700
H	8.32819100	-2.67638600	-0.64406200
H	9.06212700	-0.38253300	0.34922900
H	9.26069400	1.90835300	1.31637300
H	7.22473600	3.27620300	1.72739900
H	4.98495100	2.41065700	1.16742700
H	-8.32819300	-2.67638400	0.64404800
H	-7.15132700	-4.68277500	1.54576700
H	-4.67877200	-4.67081300	1.81542000
H	-3.34693500	-2.69289100	1.19497400
H	-4.98495000	2.41065400	-1.16745300
H	-7.22473300	3.27619300	-1.72744100
H	-9.26069100	1.90834200	-1.31641600
H	-9.06212600	-0.38253700	-0.34925800

Table S20: Coordinates of the optimized minimum in the S_1^{LE} state of QP2 at the B3LYP/cc-pVDZ level.

C	-3.25521000	0.18804100	0.01722100
S	-1.85233500	-0.93193100	0.06313400
C	-0.72304600	0.39155800	-0.00585600
C	-1.37891900	1.65110800	-0.05715800
C	-2.76142100	1.52479800	-0.04569000
C	0.69660100	0.40761700	-0.00559700
S	1.85883200	-0.90147800	0.04186000
C	3.22524200	0.23487100	-0.06004100
C	2.73136600	1.55307900	-0.10162600
C	1.33204900	1.66491500	-0.06855100
C	-4.58341200	-0.26075000	0.04296000
C	4.58352200	-0.21837800	-0.05810000
C	-5.77410300	0.54026700	-0.28104500
C	-6.93587700	-0.26278400	-0.07408900
C	-6.50177500	-1.58653700	0.36466800
C	-5.07540600	-1.59031600	0.41992600
C	5.09718400	-1.49332300	-0.48920900
C	6.55955600	-1.50914400	-0.32547600
C	6.94349600	-0.27531400	0.20383500
C	5.72559600	0.53598000	0.38059500
S	-0.03002700	2.99137700	-0.11354300
C	-0.02811700	4.11840400	1.40405100
C	-0.04514300	4.00349800	-1.70982200
H	-3.43950900	2.37397800	-0.02275000
H	3.40023600	2.40480900	-0.21308500
H	-0.02015700	3.52590800	2.33232000
H	-0.92372400	4.76208100	1.41346600
H	-0.04800900	3.34412100	-2.59187000
H	0.84304500	4.65485300	-1.76844000
H	0.85931700	4.77343000	1.40396800
H	-0.93997100	4.64665900	-1.75655100
C	-4.41774800	-2.76097300	0.83722600
C	-5.16701500	-3.89388700	1.16838300
C	-6.56748900	-3.88049000	1.09964200
C	-7.24065500	-2.72007900	0.70082800
C	-8.21466700	0.23881200	-0.31560500
C	-8.35794900	1.54967400	-0.78316000
C	-7.22326500	2.33717600	-1.02486700
C	-5.93780400	1.84221600	-0.78561500
C	7.33395000	-2.65336800	-0.68912600
C	6.69847300	-3.75322900	-1.20716200
C	5.27668000	-3.73279000	-1.38197400
C	4.48949400	-2.63961600	-1.03490900
C	5.87079600	1.81210200	0.96209500
C	7.13598500	2.26352900	1.31445500
C	8.32346900	1.48524400	1.11195300
C	8.22838000	0.22893600	0.56982400
H	-3.33258400	-2.80643000	0.92055500
H	-4.64959300	-4.80104100	1.48856100
H	-7.13414500	-4.77638400	1.36278100
H	-8.33226500	-2.70416500	0.65674600
H	-9.09534300	-0.38664100	-0.15114500
H	-9.35376900	1.95506000	-0.97518700
H	-7.34134000	3.35073800	-1.41498100
H	-5.08180500	2.47025100	-1.02705000
H	8.41750800	-2.64158900	-0.55395700
H	7.26103700	-4.64334900	-1.49200900
H	4.79211600	-4.61426900	-1.80926500
H	3.41360300	-2.68002200	-1.20181200
H	5.00261300	2.43889500	1.15943200
H	7.23464300	3.25238700	1.76942800
H	9.29056500	1.89911000	1.40085000
H	9.11703100	-0.38819300	0.42177800

Table S21: Coordinates of the optimized minimum in the S_2 state of QP2 at the B3LYP/cc-pVDZ level.

C	-3.25521400	-0.18811900	-0.01767700
S	-1.85235200	0.93185900	-0.06345300
C	-0.72308100	-0.39167000	0.00563000
C	-1.37896300	-1.65120900	0.05684400
C	-2.76145700	-1.52490900	0.04522800
C	0.69657600	-0.40766100	0.00545600
S	1.85878700	0.90145300	-0.04211800
C	3.22521300	-0.23487800	0.06008900
C	2.73135900	-1.55308700	0.10171700
C	1.33203400	-1.66493500	0.06855700
C	-4.58339300	0.26065300	-0.04324600
C	4.58346200	0.21840200	0.05828600
C	-5.77404900	-0.54026600	0.28120300
C	-6.93580100	0.26289700	0.07458700
C	-6.50173100	1.58656500	-0.36446200
C	-5.07539600	1.59019900	-0.42020400
C	5.09710600	1.49337500	0.48944800
C	6.55942700	1.50920500	0.32574000
C	6.94346700	0.27543800	-0.20366800
C	5.72556100	-0.53589100	-0.38040000
Si	-0.03000500	-2.99143700	0.11325400
C	-0.02780700	-4.11795600	-1.40474700
C	-0.04532900	-4.00415000	1.70914400
H	-3.43952200	-2.37411600	0.02213800
H	3.40025600	-2.40477600	0.21337500
H	-0.01997100	-3.52511200	-2.33279600
H	-0.92322300	-4.76189000	-1.41442300
H	-0.04910700	-3.34514000	2.59146500
H	0.84325100	-4.65494900	1.76800200
H	0.85982600	-4.77272000	-1.40489500
H	-0.93975900	-4.64791800	1.75510800
C	-4.41774300	2.76065200	-0.83808800
C	-5.16697900	3.89355600	-1.16929100
C	-6.56744700	3.88034300	-1.10002600
C	-7.24060100	2.72011300	-0.70066900
C	-8.21455600	-0.23849300	0.31674800
C	-8.35782600	-1.54928900	0.78449900
C	-7.22313000	-2.33694000	1.02572900
C	-5.93771700	-1.84217300	0.78588000
C	7.33384700	2.65341300	0.68951000
C	6.69832000	3.75321100	1.20764900
C	5.27654000	3.73273900	1.38241300
C	4.48934900	2.63958200	1.03520000
C	5.87082300	-1.81202000	-0.96192400
C	7.13603700	-2.26336700	-1.31425700
C	8.32351500	-1.48503800	-1.11179600
C	8.22838000	-0.22872100	-0.56967500
H	-3.33259100	2.80589200	-0.92186900
H	-4.64956100	4.80053600	-1.48996600
H	-7.13410700	4.77621400	-1.36322900
H	-8.33219800	2.70432700	-0.65623000
H	-9.09521000	0.38708200	0.15263900
H	-9.35361900	-1.95451400	0.97698900
H	-7.34115400	-3.35047300	1.41593700
H	-5.08168300	-2.47035800	1.02685400
H	8.41739600	2.64174500	0.55433300
H	7.26090200	4.64329100	1.49258300
H	4.79189400	4.61414000	1.80978000
H	3.41345800	2.68003300	1.20204700
H	5.00267400	-2.43886300	-1.15925200
H	7.23473600	-3.25225000	-1.76918300
H	9.29061400	-1.89887900	-1.40070400
H	9.11702700	0.38841700	-0.42168000

Table S22: Coordinates of the optimized minimum in the T_1 state of QP2 at the B3LYP/cc-pVDZ level.

C	-3.23473500	0.21066700	0.05766700
S	-1.85292200	-0.91378100	0.03742900
C	-0.72415400	0.40728600	0.01108700
C	-1.35548300	1.65625000	0.01707000
C	-2.76135700	1.53073300	0.04079600
C	0.72415700	0.40728000	-0.01091000
S	1.85291700	-0.91379700	-0.03714100
C	3.23473500	0.21064100	-0.05756700
C	2.76136900	1.53071000	-0.04067300
C	1.35549600	1.65623900	-0.01692500
C	-4.58827800	-0.25055200	0.07382900
C	4.58827500	-0.25058500	-0.07382600
C	-5.74037600	0.48574600	-0.43995100
C	-6.91841600	-0.28904100	-0.21007300
C	-6.51713600	-1.53382700	0.44787100
C	-5.09734600	-1.50817000	0.60972200
C	5.09729900	-1.50822200	-0.60971500
C	6.51710200	-1.53387500	-0.44797100
C	6.91843500	-0.28906400	0.20989500
C	5.74041300	0.48573300	0.43983100
Si	0.00001200	2.99179700	0.00006900
C	0.01944300	4.06019900	1.55850800
C	-0.01941100	4.06018500	-1.55838000
H	-3.44418900	2.37647800	0.10267500
H	3.44420700	2.37644900	-0.10259300
H	0.03249300	3.43412500	2.46438800
H	-0.87267000	4.70746700	1.59903300
H	-0.03246500	3.43410400	-2.46425400
H	0.87270700	4.70744700	-1.59890900
H	0.90976400	4.71101200	1.57493300
H	-0.90972700	4.71100300	-1.57481000
C	-4.45970600	-2.58362600	1.25243300
C	-5.22320400	-3.66855800	1.69376200
C	-6.61390600	-3.69149500	1.51525700
C	-7.26818900	-2.61737600	0.89552900
C	-8.16760400	0.17168800	-0.61836300
C	-8.25864600	1.40843800	-1.27239100
C	-7.10443900	2.16239200	-1.52922500
C	-5.84525400	1.70819700	-1.12511400
C	7.26812000	-2.61744200	-0.89564600
C	6.61378800	-3.69158200	-1.51528400
C	5.22307300	-3.66865000	-1.69368500
C	4.45960900	-2.58370000	-1.25233900
C	5.84534300	1.70821400	1.12493300
C	7.10455900	2.16242500	1.52892900
C	8.25874500	1.40845800	1.27204000
C	8.16765300	0.17168100	0.61807100
H	-3.38296700	-2.58084500	1.42395900
H	-4.72783400	-4.50611000	2.18957900
H	-7.19222400	-4.54807100	1.86830100
H	-8.35351700	-2.63256400	0.77139500
H	-9.06637800	-0.42350400	-0.44076500
H	-9.23311400	1.78051500	-1.59605000
H	-7.18733000	3.11344100	-2.05989000
H	-4.95898900	2.29407000	-1.36858000
H	8.35345700	-2.63262600	-0.77159500
H	7.19207800	-4.54817200	-1.86834100
H	4.72766400	-4.50622000	-2.18943400
H	3.38285800	-2.58092500	-1.42378400
H	4.95909600	2.29409900	1.36843800
H	7.18749100	3.11349700	2.05954700
H	9.23323900	1.78054800	1.59561000
H	9.06641300	-0.42351800	0.44042800

Table S23: Coordinates of the optimized minimum in the T_2 state of QP2 at the B3LYP/cc-pVDZ level.

C	3.22118700	0.16373700	-0.05571700
S	1.86076500	-1.01176600	-0.03873300
C	0.68875400	0.30600700	-0.01419800
C	1.34054100	1.61674300	-0.02290000
C	2.71759600	1.49327800	-0.04099600
C	-0.68875400	0.30600700	0.01420100
S	-1.86076400	-1.01176700	0.03873500
C	-3.22118700	0.16373600	0.05572000
C	-2.71759700	1.49327600	0.04099700
C	-1.34054200	1.61674200	0.02290200
C	4.58091100	-0.25663600	-0.06738300
C	-4.58091100	-0.25663700	0.06738400
C	5.71540400	0.51623000	0.43321900
C	6.91337900	-0.23093900	0.20962700
C	6.54289100	-1.49461800	-0.42818900
C	5.12159000	-1.50834500	-0.58477400
C	-5.12159200	-1.50834400	0.58477600
C	-6.54289200	-1.49461700	0.42818700
C	-6.91337700	-0.23093800	-0.20963100
C	-5.71540200	0.51623000	-0.43321900
Si	-0.00000100	2.95928300	0.00000100
C	-0.02887500	4.04686100	-1.54830500
C	0.02887400	4.04685700	1.54831100
H	3.39818900	2.34172500	-0.09676900
H	-3.39819100	2.34172200	0.09676700
H	-0.04722500	3.43411100	-2.46306500
H	0.86266400	4.69579100	-1.58530600
H	0.04720900	3.43410300	2.46306800
H	-0.86265700	4.69579800	1.58530700
H	-0.91890000	4.69894900	-1.55067300
H	0.91890800	4.69893300	1.55068900
C	4.51030400	-2.61022900	-1.21080600
C	5.30071400	-3.68085500	-1.63822900
C	6.69236600	-3.66460300	-1.46446800
C	7.32034200	-2.56416100	-0.86253800
C	8.15122000	0.26722100	0.60661100
C	8.21317800	1.51420600	1.24560200
C	7.04054100	2.24024300	1.49961000
C	5.79227400	1.74863100	1.10644900
C	-7.32034600	-2.56415900	0.86253400
C	-6.69237200	-3.66460100	1.46446600
C	-5.30072000	-3.68085400	1.63823200
C	-4.51030800	-2.61022800	1.21081000
C	-5.79226800	1.74863100	-1.10644900
C	-7.04053400	2.24024500	-1.49961400
C	-8.21317200	1.51420800	-1.24561000
C	-8.15121700	0.26722300	-0.60661800
H	3.43351800	-2.63765800	-1.37866200
H	4.82592800	-4.53831900	-2.11983000
H	7.29211700	-4.51052100	-1.80719400
H	8.40609600	-2.54926100	-0.74217200
H	9.06441800	-0.30666300	0.43256000
H	9.17901400	1.91517900	1.56033100
H	7.10020900	3.19855900	2.02010000
H	4.89362700	2.31475100	1.35058900
H	-8.40609900	-2.54925800	0.74216500
H	-7.29212500	-4.51051700	1.80719100
H	-4.82593700	-4.53831700	2.11983500
H	-3.43352300	-2.63765800	1.37866900
H	-4.89361900	2.31475000	-1.35058600
H	-7.10019900	3.19856100	-2.02010400
H	-9.17900700	1.91518300	-1.56034100
H	-9.06441600	-0.30666000	-0.43257000

Table S24: Coordinates of the optimized minimum in the S_0 state of QT1 at the B3LYP/cc-pVDZ level.

C	-3.21247900	-0.17663800	-0.00004500
S	-1.99744100	1.15675400	-0.00009900
C	-0.68935200	0.00214000	-0.00006600
C	-1.17280800	-1.35373900	-0.00006200
C	-2.53341800	-1.45265600	-0.00006500
C	0.68935600	0.00214000	-0.00005300
S	1.99744500	1.15675400	0.00000300
C	3.21248100	-0.17664000	0.00000900
C	2.53342200	-1.45265700	-0.00002300
C	1.17281100	-1.35374000	-0.00005300
C	-4.56747600	0.07163300	-0.00001500
C	4.56747900	0.07163300	0.00010700
C	-5.65442500	-0.92921900	0.00000500
C	-6.88001800	-0.25196000	0.00003800
C	-6.62908800	1.16587700	0.00004000
C	-5.24534900	1.37741700	0.00002300
C	5.24534900	1.37741600	-0.00003200
C	6.62908900	1.16587900	-0.00008400
C	6.88002000	-0.25195900	-0.00000900
C	5.65442700	-0.92921700	0.00008900
C	5.83251300	-2.34723900	0.00019500
C	7.15666500	-2.71019500	0.00015800
S	8.23499900	-1.32821400	0.00015400
S	7.52385100	2.64582100	-0.00016600
C	6.03117100	3.56755200	-0.00012200
C	4.91504200	2.76839000	-0.00003000
S	-8.23499900	-1.32821300	-0.00005300
C	-7.15666600	-2.71019500	-0.00010500
C	-5.83251400	-2.34724100	-0.00007900
C	-4.91504900	2.76839400	0.00010700
C	-6.03117900	3.56755200	0.00018400
S	-7.52385600	2.64581600	0.00014300
C	0.00000100	-2.33635600	-0.00004600
C	-0.00000700	-3.21488000	-1.26899500
C	0.00000900	-3.21482300	1.26894000
H	-3.08665700	-2.38814100	-0.00003600
H	3.08666400	-2.38814100	0.00000600
H	5.03718100	-3.09089800	0.00024100
H	7.57639500	-3.71345600	0.00007400
H	6.07775100	4.65410600	-0.00011900
H	3.90742100	3.18136200	0.00009000
H	-7.57640000	-3.71345400	-0.00013700
H	-5.03718500	-3.09090200	-0.00010700
H	-3.90743000	3.18137100	0.00010400
H	-6.07776700	4.65410500	0.00023200
H	-0.00000900	-2.59905600	-2.18071500
H	-0.89150700	-3.86188300	-1.28906800
H	-0.89148800	-3.86182900	1.28905600
H	0.00001400	-2.59896000	2.18063500
H	0.89148700	-3.86189200	-1.28907800
H	0.89151100	-3.86182300	1.28904400

Table S25: Coordinates of the optimized minimum in the S_1 state of QT1 at the B3LYP/cc-pVDZ level.

C	-3.24241000	-0.19925000	0.00178200
S	-2.02002100	1.11486000	-0.13549500
C	-0.72415000	-0.03268200	-0.02514800
C	-1.19854200	-1.36072300	0.10951800
C	-2.57791900	-1.45598800	0.12467800
C	0.68691600	-0.04287300	-0.03327800
S	2.00785800	1.09241400	-0.14713700
C	3.20094400	-0.22186700	0.02019300
C	2.54762400	-1.46235700	0.13547400
C	1.15106200	-1.36033900	0.10217100
C	-4.61068000	0.07238700	-0.01839500
C	4.60378700	0.05862500	0.00448200
C	-5.70122300	-0.90655700	0.08056900
C	-6.92619900	-0.22052600	0.02108500
C	-6.66027000	1.18336500	-0.11472600
C	-5.26830800	1.37417400	-0.14003000
C	5.26497300	1.32030700	0.18556700
C	6.71707800	1.13522900	0.10509200
C	6.96015600	-0.19168600	-0.12017300
C	5.66719700	-0.88264000	-0.19002600
C	5.85172800	-2.26162000	-0.45770300
C	7.18082400	-2.60850900	-0.57351700
S	8.32023900	-1.28269900	-0.36852600
S	7.60076900	2.64244700	0.32984000
C	6.06522400	3.47688700	0.53141400
C	4.94537000	2.67711900	0.43386300
S	-8.28885800	-1.28413700	0.12860200
C	-7.21812800	-2.66948900	0.25495400
C	-5.89232700	-2.31770400	0.21510400
C	-4.92242400	2.75662400	-0.27325400
C	-6.02618600	3.56807400	-0.34485600
S	-7.53415700	2.67147400	-0.25184300
C	-0.02250300	-2.33636500	0.20456600
C	-0.02420300	-3.33750300	-0.97010200
C	-0.01757300	-3.08443900	1.55437800
H	-3.13148100	-2.38635900	0.22257800
H	3.09265000	-2.39243100	0.28330300
H	5.05332600	-2.99090200	-0.57997200
H	7.57371100	-3.60353100	-0.77896200
H	6.07773800	4.54975700	0.71962000
H	3.93829800	3.07466500	0.54740300
H	-7.64509800	-3.66504300	0.35142700
H	-5.10161200	-3.06359700	0.28117800
H	-3.90934200	3.15421000	-0.31621300
H	-6.05744200	4.65027900	-0.44799300
H	-0.03073200	-2.81424600	-1.93798800
H	-0.91304900	-3.98717400	-0.92302800
H	-0.90679500	-3.72936300	1.64205700
H	-0.01849600	-2.37948300	2.39912700
H	0.87000500	-3.98057100	-0.93064700
H	0.87600800	-3.72398900	1.63897800

Table S26: Coordinates of the optimized minimum in the S_2 state of QT1 at the B3LYP/cc-pVDZ level.

C	-3.20094000	-0.22188500	0.02020000
S	-2.00785900	1.09245300	-0.14660900
C	-0.68691700	-0.04286300	-0.03309700
C	-1.15105400	-1.36037100	0.10188300
C	-2.54761800	-1.46240700	0.13508100
C	0.72415000	-0.03267200	-0.02503600
S	2.02001400	1.11492000	-0.13489800
C	3.24240700	-0.19923900	0.00183800
C	2.57792100	-1.45602200	0.12430700
C	1.19854500	-1.36075800	0.10916600
C	-4.60378600	0.05861200	0.00451800
C	4.61067200	0.07240100	-0.01830200
C	-5.66718500	-0.88255700	-0.19046500
C	-6.96014600	-0.19161900	-0.12036100
C	-6.71707900	1.13518200	0.10551500
C	-5.26497400	1.32021400	0.18615900
C	5.26829800	1.37412700	-0.14059300
C	6.66026200	1.18333400	-0.11516100
C	6.92619000	-0.22048500	0.02139600
C	5.70121300	-0.90648300	0.08124900
C	5.89231800	-2.31751800	0.21695600
C	7.21811800	-2.66925600	0.25722700
S	8.28884700	-1.28399500	0.12988500
S	7.53415100	2.67134000	-0.25334600
C	6.02618200	3.56787700	-0.34698400
C	4.92241700	2.75648100	-0.27482400
S	-8.32022100	-1.28252000	-0.36927800
C	-7.18080500	-2.60824800	-0.57481400
C	-5.85171400	-2.26141400	-0.45879300
C	-4.94537600	2.67690400	0.43513900
C	-6.06522900	3.47663200	0.53302700
S	-7.60076800	2.64230400	0.33093200
C	0.02251400	-2.33643400	0.20391200
C	0.02416100	-3.33714000	-0.97112500
C	0.01763300	-3.08499100	1.55345400
H	-3.09266500	-2.39251800	0.28256700
H	3.13148800	-2.38644900	0.22165200
H	5.10160600	-3.06335600	0.28368000
H	7.64508900	-3.66473200	0.35449100
H	6.05744300	4.65001300	-0.45083200
H	3.90933600	3.15403600	-0.31809300
H	-7.57370200	-3.60316200	-0.78076500
H	-5.05331000	-2.99064100	-0.58135800
H	-3.93830600	3.07437800	0.54893200
H	-6.07777500	4.54940900	0.72176500
H	0.03066200	-2.81352300	-1.93881600
H	-0.87005300	-3.98021000	-0.93187600
H	-0.87595000	-3.72456400	1.63786200
H	0.01859700	-2.38033700	2.39845300
H	0.91300100	-3.98684000	-0.92432800
H	0.90685400	-3.72995300	1.64086700

Table S27: Coordinates of the optimized minimum in the T_1 state of QT1 at the B3LYP/cc-pVDZ level.

C	-3.22117600	-0.21027000	0.01458300
S	-2.01324800	1.09893200	-0.13008300
C	-0.71924200	-0.04478200	-0.01086100
C	-1.17405200	-1.35643500	0.13004400
C	-2.57506200	-1.45332300	0.14402900
C	0.71924400	-0.04477900	-0.01085700
S	2.01324700	1.09893400	-0.13012100
C	3.22117700	-0.21026200	0.01457000
C	2.57506700	-1.45331700	0.14402100
C	1.17405700	-1.35643000	0.13005300
C	-4.61320400	0.06900800	-0.01164500
C	4.61320500	0.06901800	-0.01164000
C	-5.69486000	-0.91575600	-0.06016100
C	-6.92298200	-0.23161100	-0.05907500
C	-6.65853500	1.18210000	-0.01504300
C	-5.26533400	1.37344500	0.01160300
C	5.26534300	1.37344900	0.01162600
C	6.65854500	1.18209800	-0.01501500
C	6.92298500	-0.23161600	-0.05905400
C	5.69485700	-0.91574900	-0.06016800
C	5.87698900	-2.33270100	-0.13825000
C	7.20052700	-2.69020800	-0.18322600
S	8.27692800	-1.30275800	-0.14078200
S	7.53032500	2.67289400	0.03229700
C	6.02201000	3.57472200	0.09055500
C	4.91855900	2.76139400	0.07639200
S	-8.27694200	-1.30273900	-0.14067500
C	-7.20055900	-2.69020400	-0.18306400
C	-5.87701600	-2.33271200	-0.13812800
C	-4.91854800	2.76139500	0.07629600
C	-6.02199700	3.57472500	0.09039600
S	-7.53031400	2.67289800	0.03216200
C	0.00000400	-2.33252200	0.23713200
C	0.00001300	-3.34487500	-0.92822400
C	-0.00000100	-3.06841100	1.59414300
H	-3.12819300	-2.38117200	0.26858700
H	3.12821400	-2.38115600	0.26859500
H	5.08073600	-3.07470700	-0.17247300
H	7.62485100	-3.68983600	-0.24106100
H	6.05539600	4.66093300	0.13197600
H	3.90541500	3.15922500	0.11439500
H	-7.62489800	-3.68982800	-0.24085900
H	-5.08078100	-3.07474000	-0.17232700
H	-3.90540700	3.15923400	0.11429900
H	-6.05538500	4.66093700	0.13177400
H	0.00001600	-2.83154200	-1.90143700
H	-0.89094000	-3.99148200	-0.87842200
H	-0.89091600	-3.71046400	1.68572800
H	-0.00000700	-2.35638900	2.43296300
H	0.89096900	-3.99147700	-0.87841300
H	0.89091500	-3.71046000	1.68573600

Table S28: Coordinates of the optimized minimum in the S_0 state of QT2 at the B3LYP/cc-pVDZ level.

C	-3.22585900	-0.24182400	0.00000900
S	-1.84890700	0.90748600	-0.00004600
C	-0.69229800	-0.41196000	0.00007900
C	-2.71369700	-1.59246400	0.00011000
C	0.69229200	-0.41195100	0.00006100
S	1.84888700	0.90750800	-0.00000500
C	3.22585000	-0.24179100	0.00007300
C	2.71370300	-1.59243300	0.00005100
C	1.34951200	-1.70130200	0.00005200
C	-4.54043000	0.17481900	-0.00002900
C	4.54042400	0.17485400	0.00017900
C	-5.74618500	-0.67922800	-0.00011500
C	-6.87534700	0.14925100	-0.00006500
C	-6.44520300	1.52351800	0.00002700
C	-5.04562800	1.55549100	0.00007200
C	5.04565000	1.55551400	-0.00025300
C	6.44522700	1.52351500	-0.00039600
C	6.87534100	0.14923500	0.00004400
C	5.74615600	-0.67921400	0.00039800
C	6.10451300	-2.06282600	0.00054000
C	7.46422600	-2.25339100	0.00028700
S	8.35681700	-0.74470100	-0.00024700
S	7.14171700	3.10620700	-0.00032300
C	5.54252600	3.82839300	-0.00016200
C	4.53862500	2.89215800	-0.00011800
S	-8.35685200	-0.74463800	-0.00042500
C	-7.46430700	-2.25335300	-0.00060000
C	-6.10458800	-2.06283100	-0.00043300
C	-4.53857900	2.89212700	0.00037300
C	-5.54246300	3.82837800	0.00054100
S	-7.14166800	3.10622000	0.00034500
Si	0.00001000	-3.04532900	0.00014700
H	3.39242400	-2.44239200	-0.00004000
H	5.41059500	-2.90190500	0.00102600
H	8.00889100	-3.19469400	0.00040100
H	5.44916900	4.91193700	-0.00025000
H	3.48579900	3.17044800	-0.00001600
H	-8.00900900	-3.19463400	-0.00077300
H	-5.41070400	-2.90193600	-0.00054000
H	-3.48574800	3.17040200	0.00043900
H	-5.44909400	4.91192100	0.00070500
C	-1.34950600	-1.70131600	0.00015100
H	-3.39239400	-2.44243900	0.00020500
C	-0.00002500	-4.10522400	-1.56164200
H	0.00008900	-3.47585300	-2.46519900
H	-0.89147100	-4.75380000	-1.59207400
C	0.00005900	-4.10519300	1.56194600
H	-0.89125400	-4.75395800	1.59225200
H	-0.00009600	-3.47581900	2.46550100
H	0.89153000	-4.75373100	1.59239600
H	0.89131000	-4.75395900	-1.59196300

Table S29: Coordinates of the optimized minimum in the S_1 state of QT2 at the B3LYP/cc-pVDZ level.

C	-3.25163600	-0.27363000	0.00121800
S	-1.85867200	0.84834500	-0.08353900
C	-0.72725100	-0.47389200	0.01146100
C	-2.76405200	-1.60979800	0.09782400
C	0.69124100	-0.48987300	0.00832000
S	1.85332800	0.82007300	-0.08819600
C	3.21447200	-0.31106700	0.02700600
C	2.73016300	-1.62860700	0.11614400
C	1.33000500	-1.74309400	0.10381200
C	-4.57153100	0.18088000	-0.02885400
C	4.56763000	0.15444000	0.00537200
C	-5.78669800	-0.64234300	0.02869200
C	-6.90555100	0.20603900	-0.02823600
C	-6.44837800	1.56370600	-0.12185800
C	-5.04317000	1.56229900	-0.12332500
C	5.05416300	1.49317400	0.18897000
C	6.51724700	1.50623800	0.09989700
C	6.93550100	0.22532300	-0.13376600
C	5.74692900	-0.63376100	-0.20017200
C	6.11513000	-1.97409600	-0.47570700
C	7.47797700	-2.13752700	-0.60040400
S	8.42906200	-0.67047600	-0.39503600
S	7.19056800	3.11820400	0.32624300
C	5.55748100	3.73700800	0.53865500
C	4.55545900	2.79341600	0.44372400
S	-8.40202200	-0.66327000	0.03115000
C	-7.53275700	-2.18495400	0.13354700
C	-6.17087300	-2.01705700	0.12147900
C	-4.50855500	2.88675300	-0.21430400
C	-5.48932400	3.84370600	-0.27870600
S	-7.10737800	3.16042200	-0.23031800
Si	-0.03001100	-3.06935900	0.20335000
H	3.40380100	-2.47666700	0.22732300
H	5.42220400	-2.80434500	-0.59679400
H	8.00061200	-3.06942500	-0.81266800
H	5.42599800	4.80120900	0.73050900
H	3.50441000	3.05084200	0.56276600
H	-8.09328100	-3.11477100	0.19666100
H	-5.49024900	-2.86528400	0.17767400
H	-3.44964700	3.14104700	-0.23280000
H	-5.37070300	4.92222700	-0.35285800
C	-1.38215000	-1.73398300	0.10427500
H	-3.44884800	-2.45243700	0.16293600
C	-0.03471500	-4.24999600	-1.27245600
H	-0.03361600	-3.69147800	-2.22156800
H	-0.92876500	-4.89557600	-1.25306300
C	-0.03457300	-4.02029000	1.83646800
H	-0.92808800	-4.66246400	1.91211600
H	-0.03401400	-3.32817600	2.69303900
H	0.85492300	-4.66773700	1.91474300
H	0.85414700	-4.90278100	-1.25417900

Table S30: Coordinates of the optimized minimum in the S_2 state of QT2 at the B3LYP/cc-pVDZ level.

C	-3.21450400	-0.31109400	0.02710200
S	-1.85336700	0.82010500	-0.08785500
C	-0.69126100	-0.48981700	0.00850600
C	-2.73016500	-1.62863000	0.11606500
C	0.72725800	-0.47386200	0.01153000
S	1.85868300	0.84839900	-0.08306500
C	3.25165300	-0.27362900	0.00128100
C	2.76404700	-1.60980600	0.09752100
C	1.38214100	-1.73397900	0.10393800
C	-4.56764200	0.15444000	0.00549900
C	4.57155100	0.18090000	-0.02876700
C	-5.74694000	-0.63372800	-0.20017700
C	-6.93553000	0.22533000	-0.13369400
C	-6.51728900	1.50621100	0.10020200
C	-5.05421300	1.49313100	0.18936500
C	5.04320400	1.56227800	-0.12370600
C	6.44841700	1.56368600	-0.12214100
C	6.90558200	0.20605200	-0.02797900
C	5.78671300	-0.64230000	0.02918400
C	6.17085500	-2.01696600	0.12279400
C	7.53273300	-2.18487500	0.13513700
S	8.40203300	-0.66324700	0.03215800
S	7.10742900	3.16034400	-0.23135800
C	5.48937200	3.84360400	-0.28031700
C	4.50860200	2.88668800	-0.21545000
S	-8.42904100	-0.67044500	-0.39528100
C	-7.47791400	-2.13743900	-0.60086500
C	-6.11506900	-1.97400500	-0.47604800
C	-4.55551900	2.79330600	0.44439700
C	-5.55756600	3.73688200	0.53946700
S	-7.19062500	3.11813900	0.32680100
Si	0.02999500	-3.06937600	0.20275400
H	3.44882600	-2.45249600	0.16216400
H	5.49019000	-2.86512700	0.17944600
H	8.09325000	-3.11465900	0.19880200
H	5.37076000	4.92208700	-0.35502700
H	3.44969400	3.14095800	-0.23418400
H	-8.00049700	-3.06930500	-0.81339400
H	-5.42208700	-2.80418100	-0.59729700
H	-3.50447800	3.05070700	0.56355100
H	-5.42604400	4.80103900	0.73154100
C	-1.32999000	-1.74306000	0.10379200
H	-3.40376600	-2.47673000	0.22717500
C	0.03440200	-4.24940000	-1.27355300
H	0.03234800	-3.69043900	-2.22240300
H	-0.85407000	-4.90271200	-1.25499700
C	0.03490000	-4.02087000	1.83554200
H	-0.85498900	-4.66772700	1.91420800
H	0.03535500	-3.32899900	2.69231300
H	0.92802000	-4.66368100	1.91044400
H	0.92883300	-4.89447700	-1.25505600

Table S31: Coordinates of the optimized minimum in the T_1 state of QT2 at the B3LYP/cc-pVDZ level.

C	-3.23271100	-0.29686400	0.00338900
S	-1.85301600	0.82711200	-0.03678600
C	-0.72394400	-0.49364100	0.01186000
C	-2.75905800	-1.61991000	0.05183600
C	0.72404500	-0.49348900	0.01315000
S	1.85275300	0.82789700	-0.03212700
C	3.23202800	-0.29579000	0.01090500
C	2.75980800	-1.61878700	0.05636500
C	1.35555400	-1.74322700	0.05826100
C	-4.57314700	0.17135000	-0.01458300
C	4.57317300	0.17245800	-0.00260900
C	-5.78404900	-0.65225100	0.01463600
C	-6.90306900	0.19787200	-0.01741900
C	-6.44212000	1.56003200	-0.06689000
C	-5.03591800	1.55385300	-0.06553100
C	5.05371095	1.51722887	0.29284221
C	6.45486118	1.53306639	0.17208423
C	6.89395893	0.21479789	-0.20254780
C	5.76615120	-0.61695444	-0.31374319
C	6.12317077	-1.94354098	-0.71349252
C	7.47579693	-2.09425168	-0.88475559
S	8.36575562	-0.61293630	-0.57025735
S	7.12970303	3.08445003	0.52104550
C	5.52559273	3.73203923	0.83665392
C	4.53694934	2.79531175	0.68033175
S	-8.39675800	-0.67061200	0.01285500
C	-7.52923700	-2.19654300	0.06939300
C	-6.16768000	-2.02985500	0.06461100
C	-4.49696700	2.87981900	-0.11362600
C	-5.47510700	3.83967000	-0.14959100
S	-7.09565800	3.15792900	-0.12598500
Si	0.00038300	-3.07914100	0.10768600
H	3.44214800	-2.46458500	0.10858000
H	5.42821599	-2.76445488	-0.88328726
H	8.02013254	-2.98792400	-1.18088581
H	5.42253306	4.77675753	1.12059693
H	3.48576562	3.02942134	0.84290915
H	-8.09191100	-3.12653800	0.10286100
H	-5.48714500	-2.87918100	0.09635200
H	-3.43765700	3.13251800	-0.12203600
H	-5.35515900	4.91981700	-0.18910300
C	-1.35520500	-1.74360800	0.05725600
H	-3.43988100	-2.46763000	0.08206900
C	0.00098400	-4.20237900	-1.41117600
H	0.00146500	-3.60924100	-2.33901200
H	-0.89039200	-4.85186200	-1.41675900
C	-0.00004900	-4.08622300	1.70590000
H	-0.89095900	-4.73419600	1.75898400
H	-0.00088500	-3.42552200	2.58690100
H	0.89158800	-4.73311000	1.75998800
H	0.89209300	-4.85223800	-1.41591300